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First Principles Atomistic Model for Carbon-Doped Boron Suboxide

by Amol B Rahane, Jennifer S Dunn, and Vijay Kumar

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14. ABSTRACT
An atomistic model for the effect of carbon (C) doping on the structural reorganization of boron suboxide (B_6O) was developed from first principles density functional theory. The results indicate that it is energetically preferable for a single C atom to substitute into an oxygen (O) site rather than a B site. The lattice parameters and cell volume increase to relieve the residual stress created by the C substitution. Interstitial substitutions are not favorable for single atom substitutions. However, when 2 C atoms replace 2 neighboring O atoms within the B_6O unit cell, it becomes energetically favorable to dope an interstitial O, B, or C atom along the C-C chain. If the interstitial dopant is either B or C, a local boron carbide (B_4C)-like structure with either a C-B-C or C-C-C chain is created within the B_6O unit cell, which could serve as an intermediate phase in the transformation of B_6O into B_4C. By promoting the formation of a local B_4C-like structure, it may be possible to improve the mechanical stability and elastic properties of B_6O.

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1. Introduction

Boron suboxide (B_6O) is a particularly promising material system for lightweight armor applications. It has a high hardness, low density, high mechanical strength, high oxidation resistance (<1200 °C), and chemical inertness.[1–8] However, unlike other high-performance ceramics, boron carbide (B_4C) and B_6O display low fracture toughness[7,8] and a reduction in shear strength[9–13] under extreme high temperature and pressure environmental conditions. In addition, there remain considerable challenges associated with fully densifying stoichiometric B_6O with high crystallinity.[7,8] Theoretical predictions can enable experimentalists to prescreen prospective sintering aides by determining their thermodynamic stability and impact on the elastic moduli and deformation mechanisms.

Recent experimental observations of B_4C identified amorphous shear banding as the dominant deformation and failure mode.[9–11] To understand the mechanism by which these amorphous bands form, it is important to understand the electronic and bonding structure in these materials. However, this has been difficult to determine experimentally due to the similarity in electronic and nuclear scattering cross sections for B and C (11B and 12C isotopes).[14–16] Letsoalo[17] proposed that changes in the material hardness directly relate to the electronic charge density changes associated with the B icosahedra. Balakrishnarajan[18] confirmed this by studying the effect of C concentration on the electronic and atomistic structure of B_4C using molecular modeling. He found that the electron deficiency within the B icosahedra compensated for the strong π- antibonding interactions between the B icosahedra and its linking chain and created a driving force to reduce the C concentration and increase structural disorder. To the author's knowledge, no similar theoretical study has been conducted on the B_6O crystal structure. In the current study, we employ an ab initio density functional theory (DFT) approach to determine the effect of C doping at various sites on the energetics and structural reorganization of B_6O.

2. Computational Details

First principles density functional theory calculations using the generalized gradient approximation given by Perdew et al.[19] and the projector augmented wave method[20,21] were performed within the Vienna Ab initio Simulation Package.[22,23] The plane wave cut-off energy was set to 500 eV. The calculations were considered converged when the maximum force on each ion was less than 0.001 eV/ Å, and the change in total energy was less than 10^{-4} eV. The simulation cell consisted of a 42-atom B_6O unit cell in hexagonal representation that was sampled with a 2 × 2 × 1 k-points Monkhorst-Pack grid to obtain structural properties. We performed a full relaxation of the volume, lattice parameters, and all internal atomic coordinates.

The calculated equilibrium lattice parameters for B_6O unit cell are a = 5.393 Å and c = 12.327 Å, which are in good agreement with the experimental values of Higashi[24] (a = 5.374 Å and c = 12.331 Å) and Hubert[25] (a = 5.3902 Å and c = 12.3125 Å, c/a ratio = 2.284). Hubert's B_6O was O deficient (maximum achieved O occupancy = 0.95 at 6 GPa). Therefore, when extrapolated to ideal stoichiometry, Hubert's lattice parameters are a = 5.399 Å and c =12.306 Å. Calculations that considered the effect of C doping required a larger 2 × 2 × 1 supercell (168 atoms) to prevent the artificial interaction between defect states across the periodic boundary. The lattice parameters calculated at the Γ-point (a = 5.396 Å and c = 12.311 Å) are similar to the 3 × 3 × 3 k-points calculations (a = 5.394 Å and c = 12.318 Å). Therefore, Γ-point calculations were used to study the doped system.

3. Results and Discussion

3.1 Undoped B_6O: Structural Properties

The hexagonal representation of the 2 × 2 × 1 B_6O supercell is shown in the Figure. The small (red) and large (green) spheres represent O and B, respectively. The numbers designate the substitution sites described in the Table.

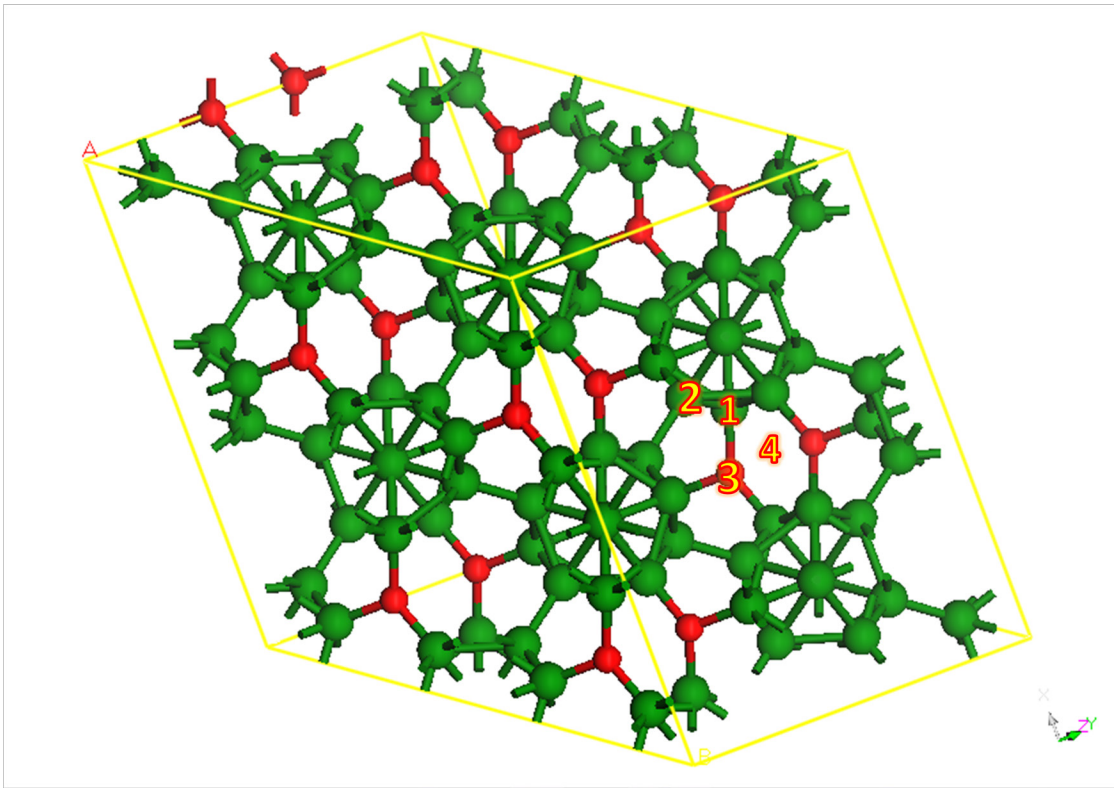

Figure Schematic representation of the B_{12} icosahedra connected by O atoms in hexagonal 2 × 2 × 1 supercell of B_6O

Table Calculated lattice parameters (Å), supercell volume (Å^3), total energy E_{total} (eV), and doping energy (eV) of undoped and C-doped B_6O configurations

Configuration	**a**	**b**	**c**	**Volume**	**E_{total}**	**E_{doping}**
2 × 2 × 1 Unit Cell	**(Å)**	**(Å)**	**(Å)**	**(Å^3)**	**(eV)**	**(eV)**
A1) Undoped B_6O	10.792	10.792	12.312	1241.94	–1197.6670	0.0
Single Carbon Atom Substitutions						
A2) Site 1: Equatorial B	10.813	10.784	12.306	1243.85	–1196.1192	+2.54
A3) Site 2: Polar B	10.791	10.791	12.307	1241.29	–1197.4815	+1.18
A4) Site 3: O	10.806	10.806	12.307	1244.56	–1197.3355	+0.05
2 Carbon Atom Substitutions						
A5) 2 Neighboring O (C_O-C_O)	10.819	10.819	12.307	1247.65	–1196.8799	+0.22
A6) 2 Polar B from adjacent B_{12}(C_P-C_P)	10.791	10.791	12.355	1245.20	–1196.8449	+2.81
A7) 1Equatorial B, 1O (C_e-C_O)	10.796	10.801	12.305	1242.46	–1198.3155	+0.06
Chain Interstitial + 2 Carbons Replacing 2 Neighboring Chain Oxygen						
A8) 2 Neighboring O + $O_{interstitial}$ (C_O-O_i-C_O)	10.810	10.834	12.316	1250.16	–1201.4684	–2.85
A9) 2 Neighboring O + $B_{interstitial}$ (C_O-B_i-C_O)	10.833	10.833	12.308	1250.82	–1203.8617	–6.52
A10) 2 Neighboring O + $C_{interstitial}$ (C_O-C_i-C_O)	10.832	10.832	12.302	1250.04	–1205.5697	–7.23
A11) 1O+$C_{interstitial}$+ 1B in O Neighbor (C_O-C_i-B_O)	10.846	10.846	12.302	1253.21	–1200.9903	–3.65
C-B-C Chain Replacing O-O Chain + Single Carbon Substitution in Neighboring B_{12} Icosahedra						
A12) $C_{equatorial}$ + C_O-B_i-C_O chain	10.822	10.819	12.311	1248.94	–1205.9958	–7.66
A13) C_{polar} + C_O-B_i-C_O chain	10.825	10.826	12.297	1248.28	–1206.2611	–7.92

The B_6O structure (space group $R\bar{3}m$) consists of 8 B_{12} icosahedral units situated at the vertices of a rhombohedral unit cell. The structure can be viewed as a distorted cubic close packing of B_{12} icosahedra. Two O atoms are located in the interstices separated by 3.07 Å along the [111] rhombohedral direction. The large O-O separation distance precludes direct O-O bonding.[25,26] Each O is bonded to 3 B from different icosahedra. The inter-icosahedral bonding creates 2 chemically distinct sites within the B icosahedra: (Site 1) B_{polar} sites through which the B-B inter-icosahedral linking occurs and (Site 2) $B_{equatorial}$ sites that form bonds with the O-O chains. This structure can also be described in terms of a hexagonal lattice based on a nonprimitive unit cell with the [0001] axis of the hexagonal lattice corresponding to the [111] rhombohedral direction. In the hexagonal representation, the unit cell of B_6O consists of 6 formula units (42 atoms).

The calculated equilibrium lattice constants are listed in the Table along with their comparison with reported values from the scientific literature. The Table lists the changes in the lattice parameters, cell volume, and energy for all C substitution sites considered in this study. Sites 2, 3, and 3 correspond to equatorial B, polar B, and O sites, respectively (see the Figure).

Negative E_{doping} values correspond to product states where the total system energy is reduced as a result of the substitution whereas positive values correspond to higher energy product states. A*) refers to the designation for the associated xyz structural file from the Appendix.

The calculated cohesive energy per atom is 6.70 eV/atom, compared with the previously reported value of 7.15 eV/atom by Lee.[27,28] There are 3 characteristic B bond lengths (L) in this system: inter-icosahedral B_{polar}-B_{polar} bonds (L = 1.70 Å), intra-icosahedral B-B bonds (L =1.76 – 1.81Å), and inter-icosahedral $B_{equatorial}$-O bonds (L = 1.50Å). The separation distance between 2 neighboring O atoms is 3.01Å. Each characteristic B bond has a unique bonding character (i.e., ionic, covalent, or metallic).

3.2 Carbon-Doped B_6O: Structural Properties

As previously noted, there are 2 chemically distinct B sites within an individual icosahedron (polar B_p and equatorial B_e). The B_p sites occupy 2 opposing 3-atom planes of the icosahedron and create B_p- B_p linkages between the icosahedra. The B_e sites bond along the equatorial axis of the icosahedron, forming a hexagonal B_e-B_e chair linkage around its circumference. In addition, each B_e atom directly bonds to the nearest neighboring O forming B_e-O chain linkages between the icosahedra. To study the effect of C on the B_6O structure, we considered the following 4 distinct C substitutions (Figure): Site 1 (C_e), C in an equatorial B site; Site 2 (C_p), C in a polar B site; Site 3 (C_O), C in an O site; and Site 4 (C_i), C as an interstitial between 2 O sites from a single O-O chain. There are 6 B_e (Site 1) and 6 B_p (Site 2) sites per icosahedra.

The calculations indicate that all single-atom C substitutions within the B_6O unit cell require additional energy, and are therefore endothermic product states. However, the difference in energy is smaller when a single C atom[29] substitutes for B in a polar site (E_{doping} = 1.18 eV) rather than a B equatorial site (E_{doping} = 2.54 eV). Each B atom in a polar site (Site 2) is coordinated to 6 neighboring B, 5 of which are from the same B_{12} icosahedra (4 B at a distance of 1.78Å and 1 B atom at 1.81Å) and 1 B atom from an adjacent icosahedra (B_p-B_p bond distance is 1.70 °A). When a single polar B is replaced by C, the lattice parameters are relatively unchanged. However, the C-B bonds shorten slightly (–2.2% for 2 C_p-B_p bonds, –1.7% for 2 C_p-B_e bonds, 0% for 1 C_p-B_e bond, and –1.1% for the inter-icosahedral C_p-B_p bond). Similarly, B in an equatorial site (Site 1) is also connected to 5 B atoms from the same B_{12} icosahedra (2 B at 1.76Å, an additional 2 B at 1.78 Å, and the final B at 1.81 Å) and 1 inter-icosahedral O atom (B_e-O bond distance is 1.50 Å). However, when a single C substitutes for an equatorial B, the a-axis lattice parameter expands (+0.2%) while the b and c axes contract –0.07% and –0.05%, respectively. This results in a +0.15% increase in the unit cell volume and an increase in the total energy of the system. The lowest energy product state for a single C substitution is when C substitutes for O (Site 3 C_O: E_{doping} = +0.05eV). During a C_O substitution, the a and b lattice parameters expand (+0.13%) while the c lattice parameter contracts (–0.04%). The substituting C atom is 4-fold coordinated to 3 equatorial B from different icosahedra (B_e-C_O bond lengths =

1.52 Å) and 1 O atom (C_O-O bond length = 3.07 Å). The B_e-C_O and C_O-O bond distances are slightly expanded compared with the neighboring B_e-O bond (1.50 Å) and O-O (3.01 Å) bond distances.

We further considered doping multiple C atoms within the B_6O structure (Table column b). The energetic cost associated with doping 2 C atoms was highest when the C substituted for 2 polar B sites from adjacent icosahedra ($E_{2Cdoping}$ = 2.81 eV). This value is nearly 2.4 times greater than the energy required to substitute a single C in a polar site ($E_{1Cdoping}$ = 1.18 eV). This is perhaps best explained by the expansion of the polar C_P-C_P inter-icosahedral bonds (from 1.7 to 2.32 Å), which precludes inter-icosahedral bonding near the C substitution. Instead, the coordination for each substituting C_p atom is satisfied by the 5 neighboring B atoms within each icosahedra. The intra-icosahedral C_p-B bond distances are in the range of 1.64–1.68 Å. There is also a +0.35% unit cell expansion along the (0001) c-axis and +0.26% unit cell volume increase. In contrast, when two C atoms replace 2 neighboring O atoms, the lattice expansion (+0.25%) occurs along the a and b lattice parameters and the C_O-C_O chain (which expands from 3.01 to 3.20 Å). The B_e-C_O bond distances are nearly identical to those that result from a single C substitution in an O site. However, the energetic cost nearly quadruples ($E_{2Cdoping}$ = 0.22 eV). The most energetically stable structure for a 2 C substitution is when the C replaces both an equatorial B and its neighboring O, forming a C_e-C_O dimer ($E_{2Cdoping}$ = 0.06 eV). The resulting structure has a C_e-C_O dimer bond distance of 1.46 Å.

3.3 Interstitial Carbon Doping in B_6O (B_4C-Like Local Structure)

According to our results, when C substitutes for 2 neighboring O sites (Site 3: C_O-C_O) within the B_6O structure, the C_O-C_O chain expands to 3.20 Å. This increase in interstitial volume suggests that it may be possible to insert a small interstitial atom (Site 4) such as O, B, or C between the 2 C_O, thereby creating a local boron carbide-like structure. There are a multitude of stable structural polytypes for boron carbide.[12–14] We explored the following candidates for an interstitial B_4C-like chain within B_6O: C-O-C, C-C-B, C-B-C, and C-C-C. We first calculated the stability of each of these interstitial chain configurations within B_6O unit cell (Table column c) and then determined the effect of an additional C substitution within a neighboring icosahedra (C_p or C_e) on their stability (Table column d).

Doping a B atom at the interstitial site along with 2 C atoms in 2 neighboring O sites creates a local B_4C-like configuration with a C-B-C chain within the B_6O unit cell. This configuration is highly energetically favorable (E_{doping} = –6.52 eV). Each C atom in this configuration is tetrahedrally coordinated to 4 B atoms. The C_O-B_e and C_O-B_i bond lengths are 1.57 and 1.44 Å, respectively. The supercell remains hexagonal although the lattice parameters expand. In contrast, if the interstitial atom is O instead of B, a significant distortion is created that acts as a driving force for a phase transformation to a triclinic B_6O unit cell. The triclinic structure is also highly stable (E_{doping} = –2.85 eV). In this relaxed configuration, the B_e-C_O and the C_O-O_i bond distances are 1.58–1.62 and 1.38 Å, respectively. We then considered interchanging 1 C_O and the

interstitial B atom within the chain, thereby forming a C_O-C_i-B_O chain. This substitution produced a slight expansion of the supercell and was much higher in energy (E_{doping} = –3.65 eV) than the C-B-C chain configuration. The C_O-C_i and C_i-B_O bond distances in C-C-B chain are 1.35 and 1.37 Å, respectively. The terminal C_O and B_O atoms in C-C-B chain are threefold coordinated to B_e atoms at distances of 1.60 and 1.65 Å, respectively. In the fourth chain configuration, the C atom is doped at an interstitial site (Site 4) in between 2 C atoms forming a C-C-C (C_O-C_i-C_O) chain with C_O-C_i and B_e-C_O bond distances of 1.32 and 1.61 Å, respectively. This substitution results in a slight expansion of the a and b lattice parameters compared with a 2 C C_O-C_O substitution. The C_O-C_i-C_O configuration is energetically more favorable than either the C-B-C chain or the C-O-C chain. The energy released is 7.23 eV for the C-C-C chain compared with 6.52 eV for the C-B-C chain and 2.85 eV for the C-O-C chain.

Finally, we considered the effect of an additional icosahedral C substitution at either an equatorial (C_e) site or polar (C_p) site on the stability of the C-B-C chain substitution (Table column d). The resultant configuration creates a local structure similar to the B_4C stoichiometry, i.e., (B_{11}C)CBC. This configuration is isoelectronic with the highly stable C-C-C configuration and the host B_6O. Doping at the polar B site (C_pCBC) is energetically more favorable than the equatorial site (C_eCBC). The lattice parameters and supercell volume decrease during both of these substitutions. The energy released is 7.92 eV for B_6O-C_pCBC compared with 7.66 eV for B_6O-C_eCBC. However, both of these configurations are more favorable than the C-C-C configuration without the icosahedral substitution (E_{doping} = –7.23 eV). The additional icosahedral C also affects the B_i-C_O bond distances in the C_O-B_i-C_O chain, which contracts from 1.44 Å for the C_O-B_i-C_O chain without the icosahedral C to 1.42–1.43 Å when C substitutes in a polar site (C_p) and expands to 1.55–1.58 Å when C substitutes in an equatorial site (C_e). The C_p atom is directly bonded to 4 B atoms at bond distances in the range of 1.68–1.75 Å and loosely bonded to 2 additional B atoms at distances of 1.77 and 1.80 Å. The B_i-C_O and B_e-C_O bond distances in the C-B-C chain of an equatorially doped C (C_eCBC) are in the range of 1.42–1.45 Å and 1.56–1.60 Å, respectively. The equatorial C atom (C_e) also forms a bond with one C atom (C_O) from the chain at a C_e-C_O bond distance equal to 1.52 Å. Experimental studies[30,31] have confirmed the existence of these intermediate phases with α-rhombohedral structures in the B-C-O system.

4. Conclusions

In summary, we calculated the structural reorganization of pure and C-doped B_6O under ambient conditions using the plane-wave pseudopotential DFT. Our calculations indicate that it is energetically preferable for C to replace O rather than B. When C replaces O, the lattice parameters and cell volume expand to relieve the residual stress created by the C substitution. The substitution product is only slightly higher in energy (E_{doping} = +0.05 eV) than undoped B_6O.

The energetic cost for C to replace 2 neighboring O more than quadruples (E_{doping} = +0.22 eV). However, if there is an interstitial (O, B, or C) between the substituting Cs, the resultant product structure is lower in energy than the system prior to substitution (E_{doping} = –7.23 to –2.85 eV). If the interstitial is either B or C, the unit cell remains tetragonal and a local B_4C-like structure is created within the B_6O unit cell. However, if the interstitial is O, a driving force is created for a transformation from the standard tetragonal B_6O unit cell to the triclinic structure. The highly exothermic nature of these product structures may explain the tendency for B_6O to form B_4C phases during processing when exposed to C contamination. In future studies, we consider the effect of these local B_4C-like structures on the electronic structure and elastic properties of B_6O.

5. References and Notes

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Appendix. XYZ Structural Coordinates for Carbon-Doped B_6O

This appendix appears in its original form, without editorial change.

Structure A1 – 2x2x1 B_6O Supercell
Gamma point optimization in VASP using high precision settings and PBE exchange functional

Total System Energy after Optimization = -1197.667069 eV
energy-cutoff : 500.00
volume of cell : 1241.94

Lattice Vectors
10.792573963 -0.000000000 0.000000000
-5.396289293 9.346641670 -0.000000000
0.000000000 -0.000000000 12.311769693

length of vectors
10.792573963 10.792573773 12.311769693

Postions in Cartsian Coordinates
B 144
O 24

168

B	-1.41588	3.93286	7.88422
B	-0.89323	3.63112	9.59390
B	3.98042	0.81728	11.98821
B	4.50307	0.51552	1.38609
B	1.28228	2.37504	3.78031
B	1.80493	2.07330	5.48999
B	-0.00052	1.48139	7.88424
B	-0.00052	2.08489	9.59391
B	2.69762	3.03915	11.98819
B	2.69762	3.64264	1.38608
B	-0.00054	4.59689	3.78032
B	2.69763	0.52708	5.48999
B	1.41485	3.93287	7.88422
B	0.89219	3.63112	9.59390
B	1.41482	0.81728	11.98820
B	0.89218	0.51552	1.38609
B	-1.28328	2.37504	3.78031
B	3.59035	2.07330	5.48999
B	4.11300	0.74072	4.42754
B	3.59035	1.04247	2.71787
B	1.41484	2.29855	8.53145
B	0.89221	2.60029	6.82178
B	-1.28333	3.85630	0.32356
B	-1.80597	4.15807	10.92568
B	1.28228	0.74073	4.42754

B	1.80493	1.04248	2.71786
B	3.98041	2.29854	8.53145
B	-0.89322	2.60029	6.82178
B	1.28227	3.85630	0.32356
B	1.80492	4.15806	10.92568
B	2.69763	3.19220	4.42753
B	2.69764	2.58870	2.71786
B	2.69759	0.07670	8.53145
B	-0.00052	4.14651	6.82178
B	-0.00052	1.63443	0.32358
B	-0.00053	1.03095	10.92568
B	3.98041	3.93286	7.88423
B	4.50306	3.63111	9.59390
B	9.37670	0.81728	11.98821
B	9.89936	0.51552	1.38609
B	6.67857	2.37503	3.78032
B	7.20122	2.07329	5.48999
B	5.39577	1.48138	7.88424
B	5.39577	2.08489	9.59391
B	8.09391	3.03915	11.98819
B	8.09390	3.64263	1.38608
B	5.39575	4.59688	3.78032
B	8.09393	0.52707	5.48999
B	6.81114	3.93286	7.88423
B	6.28848	3.63111	9.59390
B	6.81111	0.81728	11.98820
B	6.28847	0.51552	1.38609
B	4.11300	2.37504	3.78032
B	8.98665	2.07329	5.48999
B	9.50929	0.74071	4.42754
B	8.98664	1.04247	2.71787
B	6.81114	2.29854	8.53145
B	6.28850	2.60028	6.82178
B	4.11296	3.85630	0.32356
B	3.59032	4.15807	10.92567
B	6.67857	0.74072	4.42754
B	7.20122	1.04247	2.71786
B	9.37670	2.29854	8.53145
B	4.50307	2.60028	6.82178
B	6.67856	3.85629	0.32356
B	7.20121	4.15806	10.92568
B	8.09392	3.19219	4.42753
B	8.09393	2.58869	2.71786
B	8.09389	0.07670	8.53145
B	5.39578	4.14650	6.82178
B	5.39576	1.63443	0.32358

B	5.39576	1.03094	10.92569
B	-4.11406	8.60619	7.88423
B	-3.59141	8.30444	9.59390
B	1.28227	5.49060	11.98821
B	1.80491	5.18884	1.38609
B	-1.41591	7.04836	3.78031
B	-0.89327	6.74662	5.48999
B	-2.69870	6.15471	7.88423
B	-2.69870	6.75821	9.59391
B	-0.00054	7.71247	11.98819
B	-0.00053	8.31596	1.38608
B	-2.69866	9.27021	3.78032
B	-0.00055	5.20040	5.48999
B	-1.28334	8.60618	7.88423
B	-1.80599	8.30444	9.59390
B	-1.28333	5.49061	11.98820
B	-1.80598	5.18884	1.38609
B	-3.98147	7.04836	3.78032
B	0.89216	6.74662	5.48999
B	1.41481	5.41405	4.42754
B	0.89216	5.71579	2.71786
B	-1.28335	6.97187	8.53145
B	-1.80599	7.27361	6.82178
B	-3.98148	8.52962	0.32356
B	-4.50413	8.83139	10.92568
B	-1.41591	5.41404	4.42754
B	-0.89326	5.71579	2.71787
B	1.28222	6.97186	8.53145
B	-3.59142	7.27361	6.82178
B	-1.41588	8.52962	0.32357
B	-0.89324	8.83139	10.92568
B	-0.00054	7.86552	4.42753
B	-0.00055	7.26202	2.71786
B	-0.00053	4.75003	8.53144
B	-2.69870	8.81983	6.82178
B	-2.69868	6.30775	0.32358
B	-2.69868	5.70427	10.92569
B	1.28223	8.60618	7.88423
B	1.80488	8.30443	9.59390
B	6.67855	5.49060	11.98821
B	7.20120	5.18883	1.38609
B	3.98038	7.04835	3.78031
B	4.50302	6.74662	5.48999
B	2.69759	6.15470	7.88423
B	2.69759	6.75821	9.59391
B	5.39575	7.71247	11.98819

B	5.39576	8.31596	1.38608
B	2.69763	9.27020	3.78032
B	5.39574	5.20039	5.48999
B	4.11295	8.60618	7.88423
B	3.59030	8.30443	9.59391
B	4.11296	5.49060	11.98820
B	3.59030	5.18884	1.38609
B	1.41481	7.04836	3.78032
B	6.28845	6.74662	5.48999
B	6.81111	5.41404	4.42754
B	6.28845	5.71579	2.71787
B	4.11295	6.97186	8.53145
B	3.59030	7.27360	6.82178
B	1.41481	8.52962	0.32356
B	0.89215	8.83138	10.92568
B	3.98038	5.41404	4.42754
B	4.50303	5.71578	2.71787
B	6.67851	6.97187	8.53145
B	1.80487	7.27360	6.82178
B	3.98041	8.52962	0.32357
B	4.50305	8.83138	10.92568
B	5.39575	7.86552	4.42753
B	5.39574	7.26201	2.71786
B	5.39576	4.75002	8.53145
B	2.69759	8.81982	6.82178
B	2.69761	6.30775	0.32358
B	2.69761	5.70426	10.92569
O	10.79202	0.00016	7.66123
O	2.69762	1.55790	11.76560
O	-0.00051	3.11566	3.55732
O	2.69763	1.55793	8.75444
O	-0.00053	3.11568	0.54617
O	5.39574	0.00015	7.66123
O	8.09391	1.55790	11.76560
O	5.39578	3.11565	3.55733
O	8.09392	1.55793	8.75445
O	5.39576	3.11568	0.54617
O	8.09391	4.67348	7.66123
O	-0.00053	6.23122	11.76560
O	-2.69869	7.78898	3.55732
O	-0.00056	6.23125	8.75444
O	-2.69868	7.78900	0.54617
O	2.69763	4.67347	7.66122
O	5.39576	6.23122	11.76560
O	2.69760	7.78897	3.55732
O	2.69760	4.67343	4.65055

O 5.39573 6.23125 8.75444
O 2.69761 7.78900 0.54617
O 8.09389 4.67342 4.65054
O 5.39578 0.00011 4.65054
O 10.79207 0.00010 4.65054

Structure A2 – Single Carbon Substitution for an Equatorial Boron (Site 1)
Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1196.119205 eV
energy-cutoff : 500.00
volume of cell : 1243.85
direct lattice vectors
10.812928760 0.016519233 -0.007612497
-5.392159173 9.339494139 -0.000007871
-0.008654142 -0.005006886 12.306089427

length of vectors
10.812944058 10.784318769 12.306093489

Positions in Cartesian Coordinates
B 143
O 24
C 1

168

B -1.45023 3.91488 7.88830
B -0.92664 3.61337 9.60504
B 3.98026 0.81888 11.97925
B 4.51143 0.52324 1.38344
B 1.28662 2.38031 3.78026
B 1.81431 2.08664 5.49480
B -0.03118 1.45701 7.88829
B -0.03051 2.06123 9.60503
B 2.69922 3.03659 11.97199
B 2.70734 3.64608 1.37837
B 0.00826 4.59449 3.78026
B 2.70458 0.53772 5.49113
B 0.85277 3.60596 9.59655
B 1.40806 0.81208 11.98691
B 0.89313 0.51557 1.39077
B -1.28701 2.37054 3.77807
B 3.60191 2.08637 5.48803
B 4.12036 0.74873 4.42666
B 3.59634 1.04742 2.71636
B 1.37619 2.28471 8.53084

B 0.84911 2.58056 6.82247
B -1.28215 3.85364 0.32935
B -1.82340 4.14994 10.93447
B 1.28621 0.74716 4.43083
B 1.80953 1.04609 2.71953
B 3.98451 2.33492 8.50160
B -0.93411 2.57429 6.82433
B 1.29044 3.85864 0.31360
B 1.81148 4.15945 10.90468
B 2.70652 3.20308 4.42446
B 2.70250 2.59257 2.71328
B 2.69783 0.08771 8.52304
B -0.03709 4.11548 6.82248
B -0.00018 1.63322 0.32935
B -0.01419 1.01631 10.93447
B 4.01704 3.98125 7.84674
B 4.51213 3.64958 9.57049
B 9.38409 0.82450 11.98345
B 9.91856 0.52991 1.38286
B 6.69035 2.38576 3.77232
B 7.21570 2.08169 5.47877
B 5.40122 1.49094 7.87402
B 5.39253 2.09627 9.58086
B 8.10179 3.04549 11.98344
B 8.11389 3.65567 1.38286
B 5.41494 4.60751 3.77429
B 8.10634 0.53903 5.47877
B 6.82906 3.93563 7.87933
B 6.29954 3.63784 9.58716
B 6.81303 0.82077 11.97649
B 6.29854 0.52374 1.38077
B 4.12036 2.38272 3.77667
B 8.99298 2.07937 5.47160
B 9.52551 0.75122 4.41687
B 9.00165 1.05305 2.71094
B 6.81651 2.30292 8.52959
B 6.31371 2.60061 6.81616
B 4.12465 3.86110 0.31503
B 3.59556 4.15887 10.90777
B 6.69057 0.75007 4.41887
B 7.21432 1.05246 2.71015
B 9.36971 2.29687 8.53309
B 4.53022 2.61563 6.80930
B 6.69574 3.86812 0.32055
B 7.21035 4.16466 10.91942
B 8.10903 3.20464 4.41687

B	8.10849	2.60004	2.71095
B	8.09836	0.08269	8.52960
B	5.44411	4.14927	6.80918
B	5.40630	1.64321	0.31839
B	5.39537	1.03635	10.91359
B	-4.10739	8.60010	7.88107
B	-3.58517	8.30255	9.59025
B	1.28294	5.48968	11.97199
B	1.81481	5.19199	1.37836
B	-1.40638	7.04662	3.78241
B	-0.87849	6.74378	5.49112
B	-2.69441	6.15273	7.88107
B	-2.69098	6.75376	9.59025
B	0.00285	7.70795	11.97924
B	0.01239	8.31579	1.38344
B	-2.68925	9.26862	3.78240
B	0.01777	5.19833	5.49479
B	-1.27330	8.60478	7.88112
B	-1.79775	8.30200	9.58853
B	-1.28913	5.48376	11.98691
B	-1.80340	5.18610	1.39077
B	-3.97705	7.04378	3.77833
B	0.91134	6.74657	5.48802
B	1.43073	5.41278	4.42445
B	0.90001	5.71454	2.71327
B	-1.27159	6.96293	8.52303
B	-1.79821	7.27050	6.81900
B	-3.97581	8.52258	0.32669
B	-4.50803	8.81731	10.92409
B	-1.40629	5.41071	4.43083
B	-0.88575	5.71445	2.71953
B	1.31796	6.95362	8.50158
B	-3.58418	7.27060	6.81644
B	-1.40409	8.52928	0.32163
B	-0.88682	8.82791	10.91910
B	0.01215	7.86437	4.42665
B	0.00881	7.26121	2.71636
B	-0.02976	4.71988	8.53085
B	-2.69127	8.81735	6.81900
B	-2.69576	6.30546	0.32670
B	-2.70661	5.69716	10.92409
B	1.29538	8.60248	7.87402
B	1.81524	8.29232	9.58085
B	6.68892	5.49772	11.97812
B	7.22271	5.20234	1.38060
B	4.00124	7.05612	3.77429

B	4.52835	6.76218	5.48331
B	2.75990	6.15895	7.84681
B	2.72024	6.75321	9.57048
B	5.40918	7.71430	11.97811
B	5.42026	8.32429	1.38060
B	2.71485	9.27152	3.77231
B	5.42393	5.21098	5.48332
B	4.12642	8.61670	7.87933
B	3.60378	8.30703	9.58715
B	4.11634	5.49016	11.97453
B	3.60270	5.19363	1.37970
B	1.42721	7.04738	3.77667
B	6.31344	6.75867	5.47863
B	6.83423	5.42658	4.41798
B	6.30934	5.72632	2.71033
B	4.13953	6.99216	8.51948
B	3.61897	7.31049	6.80919
B	1.42975	8.53079	0.31838
B	0.89875	8.82473	10.91359
B	4.00180	5.42404	4.42435
B	4.52218	5.72448	2.71039
B	6.70438	6.98437	8.51892
B	1.83388	7.28584	6.80932
B	4.00131	8.53503	0.32054
B	4.51543	8.83239	10.91942
B	5.42021	7.87573	4.41798
B	5.41735	7.27130	2.71033
B	5.42873	4.75929	8.51950
B	2.71260	8.83791	6.81615
B	2.70968	6.31191	0.31503
B	2.70302	5.70480	10.90777
O	5.41335	9.35091	7.65451
O	2.69181	1.55389	11.75443
O	-0.00086	3.11309	3.55693
O	2.68514	1.58870	8.71783
O	0.00573	3.11692	0.54373
O	0.00797	9.34453	7.65571
O	8.09980	1.56367	11.75914
O	5.40590	3.12385	3.55121
O	8.09719	1.56220	8.76681
O	5.41076	3.12571	0.54088
O	8.10832	4.68302	7.65451
O	-0.00484	6.22460	11.75443
O	-2.69087	7.78635	3.56023
O	0.02192	6.20145	8.71783
O	-2.68943	7.78720	0.54739

O 2.88039 4.77625 7.50258
O 5.40279 6.23288 11.75622
O 2.71184 7.79010 3.55121
O 2.71609 4.68174 4.62723
O 5.42530 6.24587 8.73784
O 2.71586 7.79341 0.54088
O -2.69264 4.66978 4.65061
O 5.40597 0.00842 4.64652
O 0.00137 0.00363 4.65062
C 1.17911 3.79438 7.93568

Structure A3 – Single Carbon Substitution for a Polar Boron (Site 2)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1197.481537 eV
energy-cutoff : 500.00
volume of cell : 1241.29
direct lattice vectors
10.790562268 0.002284302 0.012507432
-5.393302653 9.346043381 -0.012507591
0.014218978 -0.008209344 12.306937056

length of vectors
10.790569759 10.790569810 12.306948008

Positions in Cartesian Coordinates
B 143
O 24
C 1

168

B -1.39257 3.91993 7.87343
B -0.87253 3.61969 9.57946
B 3.99471 0.80959 11.99229
B 4.49726 0.51944 1.40089
B 1.26728 2.38427 3.79972
B 1.77741 2.08975 5.54410
B 0.02101 1.46931 7.87300
B 0.01900 2.07294 9.58073
B 2.71315 3.03066 11.98848
B 2.69418 3.64537 1.39601
B 0.00014 4.60357 3.76205
B 2.67891 0.53990 5.51600
B 1.43652 3.92105 7.87300
B 0.91276 3.62098 9.58073

B	1.43042	0.80892	11.98848
B	0.88858	0.51799	1.39601
B	-1.28826	2.37200	3.76205
B	3.57037	2.08395	5.51600
B	4.09886	0.74946	4.45334
B	3.58240	1.04763	2.73757
B	1.43757	2.28595	8.53475
B	-1.28189	3.85603	0.31795
B	-1.78890	4.14876	10.91586
B	1.26642	0.74781	4.45123
B	1.79754	1.04836	2.73717
B	4.00831	2.29875	8.52839
B	-0.86744	2.58870	6.79950
B	1.28267	3.85661	0.32227
B	1.82796	4.15031	10.91932
B	2.68406	3.20324	4.45123
B	2.68935	2.59301	2.73717
B	2.71185	0.05323	8.52839
B	0.02288	4.13078	6.79950
B	-0.00011	1.63477	0.32227
B	0.01819	1.01569	10.91932
B	4.00810	3.92227	7.88621
B	4.52015	3.62419	9.59649
B	9.38991	0.80983	11.99062
B	9.89571	0.51691	1.39347
B	6.67791	2.37380	3.79220
B	7.21542	2.07161	5.49471
B	5.41153	1.47702	7.88587
B	5.41117	2.07730	9.59794
B	8.10833	3.03191	11.98852
B	8.09247	3.64529	1.39083
B	5.39752	4.59906	3.78299
B	8.09854	0.52628	5.49092
B	6.82044	3.92325	7.88334
B	6.30333	3.62421	9.59440
B	6.82203	0.80977	11.99302
B	6.28260	0.51786	1.39639
B	4.09996	2.37941	3.80557
B	8.99933	2.06525	5.47631
B	9.50257	0.73794	4.42280
B	8.97905	1.04277	2.71732
B	6.82033	2.29578	8.52804
B	6.29936	2.59727	6.82460
B	4.11255	3.85696	0.32986
B	3.60638	4.15049	10.92759
B	6.67911	0.74286	4.43899

B	7.19504	1.04290	2.72451
B	9.39742	2.29264	8.52690
B	4.52045	2.59947	6.83063
B	6.67939	3.85796	0.32647
B	7.21914	4.15082	10.92550
B	8.09550	3.19112	4.42904
B	8.08712	2.58897	2.71898
B	8.10775	0.06273	8.53049
B	5.41051	4.14251	6.82165
B	5.39327	1.63624	0.33306
B	5.40919	1.02194	10.93185
B	-4.08756	8.58770	7.87370
B	-3.57339	8.29328	9.58398
B	1.29880	5.48313	11.97812
B	1.80537	5.19155	1.38096
B	-1.41164	7.04980	3.77969
B	-0.88118	6.73541	5.48221
B	-2.68224	6.15165	7.87083
B	-2.68181	6.74900	9.58189
B	0.01491	7.70701	11.98051
B	-0.00201	8.32012	1.38388
B	-2.70548	9.27957	3.79306
B	0.01629	5.19367	5.46380
B	-1.26819	8.59491	7.87337
B	-1.78824	8.29509	9.58544
B	-1.26637	5.48197	11.97602
B	-1.80550	5.18902	1.37832
B	-3.97897	7.04603	3.77048
B	0.89867	6.74326	5.47842
B	1.41739	5.42151	4.41030
B	0.89164	5.72247	2.70481
B	-1.27286	6.96548	8.51553
B	-1.79445	7.26590	6.81210
B	-3.97877	8.52989	0.31735
B	-4.48606	8.82149	10.91508
B	-1.41066	5.41347	4.41654
B	-0.89338	5.72181	2.70648
B	1.30473	6.96707	8.51798
B	-3.57709	7.26305	6.80915
B	-1.41522	8.53112	0.32055
B	-0.87525	8.82448	10.91934
B	0.00140	7.86424	4.42649
B	-0.00048	7.26741	2.71201
B	0.01840	4.73522	8.51439
B	-2.68581	8.80539	6.81812
B	-2.69622	6.30644	0.31397

B	-2.67997	5.69258	10.91299
B	1.30111	8.59696	7.87553
B	1.82201	8.29622	9.58621
B	6.69525	5.48265	11.98526
B	7.20238	5.18985	1.38797
B	3.98536	7.04721	3.77875
B	4.51213	6.74308	5.48259
B	2.71091	6.15507	7.87059
B	2.71494	6.74933	9.58366
B	5.41164	7.70584	11.98506
B	5.39561	8.31854	1.38788
B	2.69619	9.27035	3.77206
B	5.40105	5.20194	5.48693
B	4.12074	8.59698	7.87059
B	3.60812	8.29636	9.58366
B	4.12811	5.48269	11.98506
B	3.58948	5.19022	1.38788
B	1.41548	7.05209	3.77206
B	6.29125	6.74381	5.48693
B	6.81144	5.41557	4.42646
B	6.29089	5.71611	2.71612
B	4.12615	6.96592	8.51923
B	3.60186	7.26862	6.81346
B	1.41451	8.53149	0.32123
B	0.90709	8.82444	10.91964
B	3.98901	5.41809	4.42618
B	4.50612	5.71606	2.71551
B	6.69489	6.96408	8.53079
B	1.82033	7.26827	6.81163
B	3.98148	8.53043	0.32038
B	4.52152	8.82308	10.91942
B	5.39804	7.85861	4.42618
B	5.39855	7.26179	2.71551
B	5.41211	4.74225	8.53079
B	2.71140	8.81164	6.81163
B	2.69891	6.30896	0.32038
B	2.71549	5.69494	10.91942
O	0.02381	0.00786	7.63655
O	2.71174	1.55031	11.76197
O	-0.00499	3.11882	3.54263
O	2.70156	1.55619	8.71540
O	0.00027	3.11578	0.54323
O	0.01559	9.33915	7.65133
O	8.10706	1.55015	11.76741
O	5.38871	3.11260	3.57835
O	8.11782	1.55535	8.73947

O 5.39591 3.11843 0.55293
O -2.67103 4.65805 7.64374
O 0.01624 6.22395 11.75490
O -2.69606 7.79689 3.56584
O 0.01712 6.21204 8.72697
O -2.69751 7.78773 0.54042
O 2.70358 4.64935 7.63655
O 5.41181 6.22364 11.76328
O 2.70052 7.78901 3.55048
O 2.69802 4.68201 4.65038
O 5.40966 6.22488 8.75137
O 2.69830 7.79029 0.54353
O 8.09784 4.67287 4.65227
O 5.38786 0.00525 4.67025
O 5.39001 9.34467 4.65038
C 0.87439 2.61111 6.85654

Structure A4 – Single Carbon Substitution for an Oxygen (Site 3)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1197.335571 eV
energy-cutoff : 500.00
volume of cell : 1244.56
direct lattice vectors
10.806031269 -0.000003798 0.000004258
-5.403018873 9.358294170 -0.000004597
0.000004923 -0.000003185 12.307001153

length of vectors
10.806031269 10.806029924 12.307001153
Positions in Cartesian Coordinates
B 144
O 23
C 1

168

B -1.43070 3.93384 7.88692
B -0.90069 3.63820 9.58985
B 3.98501 0.81789 11.98406
B 4.50891 0.51670 1.38616
B 1.28467 2.37812 3.78246
B 1.80429 2.06827 5.49126
B -0.01044 1.47387 7.88692
B -0.00146 2.08070 9.58985
B 2.70098 3.04373 11.98188

B	2.70098	3.64799	1.38562
B	-0.00003	4.60328	3.78246
B	2.70098	0.52442	5.48644
B	1.38988	3.92233	7.86760
B	0.88862	3.63292	9.58651
B	1.41696	0.81789	11.98406
B	0.89305	0.51670	1.38616
B	-1.28462	2.37818	3.77695
B	3.59767	2.06827	5.49126
B	4.11727	0.74035	4.42387
B	3.59424	1.04639	2.71635
B	1.40171	2.28521	8.51509
B	0.88137	2.58243	6.82015
B	-1.28489	3.86104	0.32380
B	-1.80853	4.16375	10.92216
B	1.28470	0.74035	4.42387
B	1.80772	1.04639	2.71635
B	4.00024	2.28521	8.51509
B	-0.90152	2.59938	6.81615
B	1.28438	3.86140	0.32194
B	1.80489	4.16192	10.91781
B	2.70098	3.19437	4.43574
B	2.70098	2.59547	2.71970
B	2.70098	0.07850	8.52604
B	-0.02475	4.15187	6.82015
B	-0.00057	1.63653	0.32380
B	-0.00023	1.03170	10.92216
B	4.01203	3.92234	7.86759
B	4.51334	3.63292	9.58651
B	9.38836	0.81832	11.98521
B	9.91281	0.51552	1.38650
B	6.68659	2.37818	3.77695
B	7.21065	2.07561	5.48583
B	5.41239	1.47387	7.88692
B	5.40341	2.08070	9.58985
B	8.10400	3.04289	11.98520
B	8.10399	3.64847	1.38650
B	5.40199	4.60328	3.78246
B	8.10400	0.52829	5.48584
B	6.83266	3.93384	7.88692
B	6.30264	3.63820	9.58985
B	6.81964	0.81832	11.98520
B	6.29518	0.51552	1.38650
B	4.11729	2.37812	3.78246
B	8.99735	2.07561	5.48583
B	9.52138	0.74151	4.42401

B	8.99783	1.04378	2.71583
B	6.82261	2.29966	8.53052
B	6.30348	2.59937	6.81615
B	4.11757	3.86140	0.32194
B	3.59706	4.16193	10.91780
B	6.68662	0.74151	4.42401
B	7.21017	1.04378	2.71583
B	9.38537	2.29965	8.53052
B	4.52059	2.58243	6.82015
B	6.68685	3.86104	0.32380
B	7.21048	4.16375	10.92216
B	8.10400	3.19649	4.42400
B	8.10400	2.59194	2.71583
B	8.10399	0.08025	8.53052
B	5.42671	4.15187	6.82015
B	5.40253	1.63653	0.32381
B	5.40219	1.03170	10.92216
B	-4.11791	8.61617	7.88052
B	-3.59561	8.31462	9.58913
B	1.28456	5.49705	11.98189
B	1.80786	5.19491	1.38562
B	-1.41794	7.05732	3.77620
B	-0.89723	6.75670	5.48644
B	-2.70204	6.16381	7.88053
B	-2.70204	6.76691	9.58914
B	-0.00107	7.72197	11.98405
B	0.00005	8.32627	1.38616
B	-2.70204	9.28145	3.77620
B	-0.00856	5.20822	5.49126
B	-1.28617	8.61617	7.88052
B	-1.80847	8.31462	9.58913
B	-1.28509	5.49797	11.98405
B	-1.80788	5.19485	1.38616
B	-3.98614	7.05733	3.77620
B	0.88813	6.76132	5.49126
B	1.41502	5.42172	4.43574
B	0.89636	5.72116	2.71970
B	-1.28343	6.97968	8.52604
B	-1.80973	7.28354	6.81784
B	-3.98649	8.54028	0.32354
B	-4.50958	8.84229	10.92136
B	-1.41837	5.42219	4.42386
B	-0.89182	5.72212	2.71635
B	1.27728	7.00152	8.51509
B	-3.59435	7.28354	6.81784
B	-1.41759	8.54028	0.32355

B	-0.89450	8.84229	10.92136
B	-0.00209	7.87526	4.42386
B	0.00144	7.26929	2.71635
B	-0.02198	4.75113	8.51509
B	-2.70204	8.82906	6.81784
B	-2.70204	6.31556	0.32355
B	-2.70204	5.71155	10.92136
B	1.28071	8.63015	7.88692
B	1.80175	8.31896	9.58985
B	6.68706	5.49797	11.98406
B	7.20984	5.19484	1.38616
B	3.98567	7.05640	3.78246
B	4.51383	6.76132	5.49126
B	2.70097	6.19319	7.86760
B	2.70097	6.77202	9.58652
B	5.40303	7.72197	11.98405
B	5.40190	8.32627	1.38616
B	2.70098	9.28144	3.77695
B	5.41051	5.20822	5.49126
B	4.12124	8.63015	7.88692
B	3.60020	8.31896	9.58985
B	4.11740	5.49705	11.98188
B	3.59409	5.19491	1.38562
B	1.41628	7.05640	3.78246
B	6.29919	6.75670	5.48644
B	6.82033	5.42219	4.42387
B	6.29377	5.72212	2.71635
B	4.12467	7.00152	8.51509
B	3.60709	7.30353	6.82015
B	1.41665	8.54026	0.32380
B	0.89268	8.84239	10.92216
B	3.98694	5.42171	4.43574
B	4.50560	5.72116	2.71970
B	6.68538	6.97968	8.52604
B	1.79486	7.30353	6.82015
B	3.98530	8.54025	0.32380
B	4.50927	8.84238	10.92216
B	5.40404	7.87526	4.42386
B	5.40051	7.26929	2.71635
B	5.42394	4.75113	8.51509
B	2.70098	8.83909	6.81615
B	2.70098	6.31502	0.32194
B	2.70098	5.71399	10.91781
O	5.40303	9.35812	7.65916
O	2.70099	1.55935	11.76293
O	-0.00035	3.11965	3.56004

O 2.70097 1.56189 8.73816
O -0.00069 3.11947 0.54578
O -0.00107 9.35812 7.65916
O 8.10400 1.55984 11.76338
O 5.40232 3.11965 3.56004
O 8.10399 1.55985 8.74022
O 5.40264 3.11947 0.54578
O 8.10400 4.67991 7.65916
O -0.00095 6.23924 11.76293
O -2.70203 7.79870 3.55173
O 0.00123 6.23798 8.73816
O -2.70204 7.79871 0.54548
O 5.40292 6.23923 11.76293
O 2.70098 7.79850 3.56004
O 2.70098 4.67927 4.67610
O 5.40072 6.23798 8.73816
O 2.70097 7.79889 0.54578
O 8.10400 4.67931 4.64510
O 5.40245 0.00009 4.64510
O 10.80555 0.00009 4.64511
C 2.70101 4.67928 7.74810

Structure A5 – Two Carbon Atoms Replacing Two Adjacent Oxygen Atoms
Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1196.879945 eV
energy-cutoff : 500.00
volume of cell : 1247.65
direct lattice vectors
10.819544375 -0.000002183 -0.000000118
-5.409774016 9.369999231 0.000000127
-0.000000071 0.000000028 12.306785239

length of vectors
10.819544375 10.819544375 12.306785239

Positions in Cartesian Coordinates
B 144
O 22
C 2

168

B -1.43290 3.93740 7.88864
B -0.90078 3.64280 9.59070
B 3.99008 0.81919 11.98295
B 4.51493 0.51685 1.38435

B	1.27894	2.35875	3.79272
B	1.79576	2.05275	5.48836
B	-0.01183	1.47603	7.88864
B	-0.00090	2.08417	9.59070
B	2.70436	3.04823	11.98336
B	2.70435	3.65020	1.38900
B	-0.02306	4.61387	3.79272
B	2.70436	0.51740	5.48772
B	1.38963	3.92608	7.86417
B	0.89068	3.63801	9.58558
B	1.41863	0.81919	11.98295
B	0.89379	0.51685	1.38435
B	-1.28508	2.38183	3.77815
B	3.61295	2.05275	5.48836
B	4.12543	0.72828	4.41813
B	3.60425	1.04183	2.71606
B	1.40236	2.28752	8.51407
B	0.87898	2.58208	6.81841
B	-1.28652	3.86561	0.32380
B	-1.81076	4.16897	10.92239
B	1.28329	0.72829	4.41813
B	1.80446	1.04183	2.71606
B	4.00634	2.28752	8.51407
B	-0.90497	2.60129	6.81903
B	1.28674	3.86667	0.32361
B	1.80807	4.16767	10.91795
B	2.70435	3.16700	4.44261
B	2.70436	2.59084	2.72126
B	2.70435	0.07854	8.52864
B	-0.02963	4.15584	6.81841
B	-0.00081	1.63869	0.32381
B	-0.00021	1.03301	10.92239
B	4.01907	3.92608	7.86417
B	4.51802	3.63801	9.58558
B	9.40013	0.81933	11.98521
B	9.92532	0.51610	1.38667
B	6.69379	2.38183	3.77815
B	7.21975	2.07816	5.48734
B	5.42053	1.47603	7.88864
B	5.40961	2.08417	9.59070
B	8.11413	3.04674	11.98520
B	8.11413	3.65318	1.38667
B	5.43176	4.61387	3.79272
B	8.11413	0.52906	5.48734
B	6.84161	3.93740	7.88864
B	6.30948	3.64280	9.59070

B	6.82813	0.81933	11.98520
B	6.30294	0.51610	1.38667
B	4.12977	2.35875	3.79272
B	9.00850	2.07816	5.48734
B	9.53213	0.74311	4.42482
B	9.00893	1.04518	2.71664
B	6.83153	2.30231	8.53374
B	6.31367	2.60129	6.81903
B	4.12197	3.86667	0.32361
B	3.60063	4.16767	10.91795
B	6.69613	0.74311	4.42482
B	7.21933	1.04518	2.71664
B	9.39672	2.30230	8.53374
B	4.52973	2.58208	6.81841
B	6.69523	3.86561	0.32380
B	7.21947	4.16897	10.92239
B	8.11413	3.19916	4.42482
B	8.11413	2.59502	2.71664
B	8.11413	0.08079	8.53374
B	5.43834	4.15584	6.81841
B	5.40952	1.63869	0.32381
B	5.40892	1.03301	10.92239
B	-4.12341	8.62714	7.88198
B	-3.60022	8.32508	9.59013
B	1.28675	5.50358	11.98337
B	1.80808	5.20259	1.38900
B	-1.42282	7.06795	3.77296
B	-0.90501	6.76900	5.48772
B	-2.70542	6.17112	7.88198
B	-2.70542	6.77524	9.59013
B	-0.00079	7.73158	11.98295
B	-0.00020	8.33727	1.38435
B	-2.70542	9.28948	3.77296
B	-0.02966	5.21445	5.48836
B	-1.28743	8.62714	7.88198
B	-1.81062	8.32508	9.59013
B	-1.28652	5.50463	11.98295
B	-1.81076	5.20127	1.38435
B	-3.98802	7.06795	3.77296
B	0.87894	6.78819	5.48836
B	1.38961	5.44419	4.44261
B	0.89065	5.73227	2.72126
B	-1.28507	6.98843	8.52864
B	-1.81105	7.29210	6.81945
B	-3.99143	8.55094	0.32151
B	-4.51663	8.85417	10.92007

B	-1.43291	5.43287	4.41813
B	-0.90078	5.72745	2.71606
B	1.27895	7.01150	8.51407
B	-3.59979	7.29210	6.81945
B	-1.41940	8.55094	0.32151
B	-0.89421	8.85417	10.92007
B	-0.01184	7.89423	4.41813
B	-0.00089	7.28611	2.71606
B	-0.02304	4.75639	8.51407
B	-2.70542	8.84119	6.81945
B	-2.70542	6.32350	0.32151
B	-2.70542	5.71706	10.92007
B	1.28328	8.64196	7.88864
B	1.80448	8.32844	9.59070
B	6.69523	5.50463	11.98295
B	7.21947	5.20127	1.38435
B	4.00635	7.08276	3.79272
B	4.52976	6.78819	5.48836
B	2.70435	6.20324	7.86417
B	2.70435	6.77938	9.58558
B	5.40950	7.73158	11.98295
B	5.40890	8.33727	1.38435
B	2.70435	9.29172	3.77815
B	5.43836	5.21445	5.48836
B	4.12543	8.64196	7.88864
B	3.60422	8.32844	9.59070
B	4.12196	5.50358	11.98337
B	3.60063	5.20259	1.38900
B	1.40236	7.08276	3.79272
B	6.31371	6.76899	5.48772
B	6.84162	5.43287	4.41813
B	6.30949	5.72744	2.71606
B	4.12975	7.01150	8.51407
B	3.61296	7.31748	6.81841
B	1.41864	8.55109	0.32380
B	0.89380	8.85341	10.92239
B	4.01909	5.44419	4.44261
B	4.51806	5.73227	2.72126
B	6.69378	6.98843	8.52864
B	1.79574	7.31748	6.81841
B	3.99007	8.55109	0.32380
B	4.51490	8.85341	10.92239
B	5.42055	7.89423	4.41813
B	5.40960	7.28611	2.71606
B	5.43174	4.75639	8.51407
B	2.70435	8.85281	6.81903

B 2.70435 6.32205 0.32361
B 2.70435 5.72007 10.91795
O 0.00004 -0.00020 7.66242
O 2.70436 1.56138 11.76254
O 0.00119 3.12445 3.57183
O 2.70435 1.56379 8.73494
O -0.00092 3.12324 0.54432
O 5.40867 -0.00020 7.66242
O 8.11413 1.56180 11.76423
O 5.40752 3.12445 3.57183
O 8.11413 1.56180 8.74464
O 5.40963 3.12324 0.54432
O -2.70542 4.68580 7.66242
O -0.00089 6.24700 11.76254
O -2.70542 7.80846 3.56204
O 0.00119 6.24581 8.73494
O -2.70542 7.80846 0.54239
O 5.40960 6.24700 11.76254
O 2.70435 7.80648 3.57183
O 5.40752 6.24580 8.73495
O 2.70436 7.80891 0.54432
O 8.11413 4.68447 4.64438
O 5.40981 0.00045 4.64438
O 10.81845 0.00045 4.64438
C 2.70435 4.68513 7.75581
C 2.70435 4.68513 4.55097

Structure A6 – Two Carbons Replacing Two Boron Atoms in Polar Sites from Adjacent B_{12} Icosahedra

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1196.844191 eV
energy-cutoff : 500.00
volume of cell : 1245.20
direct lattice vectors
10.791068870 -0.005683755 -0.022831780
-5.400456633 9.342497964 0.022831679
-0.026074952 0.015054255 12.355057690

length of vectors
10.791094521 10.791094538 12.355094377

Positions in Cartesian Coordinates
B 142
O 24
C 2

168

B -1.46281 3.95665 7.95170
B -0.93248 3.65046 9.65675
B 3.95431 0.82908 12.01839
B 4.51114 0.50759 1.37063
B 1.32341 2.34803 3.73175
B -0.04670 1.52817 7.96469
B -0.04992 2.10370 9.68000
B 2.67034 3.05343 12.02406
B 2.70656 3.64163 1.36827
B 0.00536 4.58655 3.81010
B 2.71009 0.52805 5.46517
B 1.34837 3.94451 7.96469
B 0.84833 3.65953 9.68000
B 1.38598 0.82884 12.02406
B 0.89469 0.50338 1.36827
B -1.27423 2.37023 3.81010
B 3.59290 2.05711 5.46517
B 4.13098 0.72708 4.40336
B 3.60065 1.03326 2.69831
B 1.34476 2.33570 8.62331
B -1.28613 3.85465 0.33667
B -1.84296 4.17613 10.98443
B 1.31979 0.73922 4.39037
B 1.81984 1.02420 2.67506
B 3.94240 2.31349 8.54496
B -0.92473 2.62662 6.88989
B 1.28220 3.85488 0.33100
B 1.77349 4.18034 10.98678
B 2.71487 3.15556 4.39037
B 2.71809 2.58002 2.67506
B 2.66281 0.09718 8.54496
B -0.04193 4.15568 6.88989
B -0.00217 1.63029 0.33100
B -0.03839 1.04209 10.98678
B 3.94372 3.93825 7.89770
B 4.46170 3.64305 9.61595
B 9.34522 0.82368 12.02194
B 9.90318 0.50521 1.37532
B 6.69335 2.36973 3.78096
B 7.20138 2.07278 5.49904
B 5.35913 1.49399 7.90158
B 5.35450 2.09528 9.61690
B 8.06210 3.04833 12.02199
B 8.09241 3.63523 1.37948
B 5.39460 4.59316 3.78876
B 8.09621 0.52831 5.49571

B	6.76811	3.94009	7.90475
B	6.24805	3.64081	9.61889
B	6.78398	0.82801	12.01583
B	6.29432	0.51048	1.37644
B	4.13380	2.36367	3.75665
B	8.99341	2.06920	5.49264
B	9.51551	0.73980	4.43453
B	8.99754	1.03499	2.71627
B	6.76589	2.30832	8.55126
B	6.25785	2.60526	6.83318
B	4.11402	3.85436	0.31028
B	3.55607	4.17283	10.95691
B	6.69113	0.73795	4.42747
B	7.21119	1.03723	2.71333
B	9.32544	2.31437	8.57558
B	4.46582	2.60884	6.83959
B	6.67527	3.85003	0.31639
B	7.16492	4.16756	10.95578
B	8.10010	3.18405	4.43064
B	8.10474	2.58276	2.71532
B	8.06464	0.08489	8.54346
B	5.36302	4.14973	6.83651
B	5.39715	1.62970	0.31024
B	5.36684	1.04281	10.95274
B	-4.14406	8.62615	7.92053
B	-3.62942	8.32517	9.63879
B	1.25398	5.50560	12.04477
B	1.80876	5.18164	1.39815
B	-1.41087	7.02917	3.80380
B	-0.89969	6.73767	5.52187
B	-2.73347	6.17924	7.92759
B	-2.73431	6.77927	9.64173
B	-0.03038	7.72155	12.03866
B	-0.00023	8.30436	1.39927
B	-2.68540	9.24883	3.77948
B	-0.00057	5.18752	5.51547
B	-1.31957	8.62250	7.92441
B	-1.84262	8.32587	9.63973
B	-1.31418	5.50449	12.04482
B	-1.80730	5.18480	1.40231
B	-3.98579	7.04221	3.81159
B	0.88528	6.73496	5.51855
B	1.41177	5.40007	4.45736
B	0.89714	5.70105	2.73910
B	-1.32142	6.99705	8.57409
B	-1.83260	7.28856	6.85601

B	-3.98626	8.52062	0.33312
B	-4.54104	8.84458	10.97974
B	-1.41272	5.40372	4.45348
B	-0.88966	5.70036	2.73816
B	1.25351	6.98402	8.56629
B	-3.61757	7.29126	6.85935
B	-1.41809	8.52173	0.33307
B	-0.92498	8.84142	10.97558
B	0.00118	7.84698	4.45031
B	0.00202	7.24696	2.73616
B	-0.04689	4.77739	8.59841
B	-2.73171	8.83870	6.86242
B	-2.70189	6.30468	0.33923
B	-2.73205	5.72186	10.97861
B	1.25290	8.61328	7.91714
B	1.77398	8.31243	9.63286
B	6.64707	5.49895	12.02418
B	7.19749	5.18117	1.38338
B	3.97667	7.04071	3.79334
B	4.49024	6.74420	5.50478
B	2.66435	6.16073	7.91656
B	2.66729	6.76591	9.63038
B	5.36275	7.71767	12.02548
B	5.39343	8.30232	1.38468
B	2.70162	9.26271	3.80692
B	5.38548	5.19837	5.49904
B	4.08259	8.61720	7.91656
B	3.55996	8.31206	9.63038
B	4.08344	5.50185	12.02548
B	3.59246	5.18296	1.38468
B	1.41484	7.03393	3.80692
B	6.27659	6.74181	5.49904
B	6.80588	5.40726	4.43792
B	6.28480	5.70811	2.72220
B	4.08211	6.97983	8.56172
B	3.56855	7.27634	6.85028
B	1.41172	8.52158	0.33088
B	0.86130	8.83937	10.97168
B	3.97619	5.40334	4.43849
B	4.49882	5.70848	2.72468
B	6.64394	6.98661	8.54814
B	1.78219	7.27873	6.85602
B	3.97535	8.51869	0.32958
B	4.46633	8.83758	10.97038
B	5.39443	7.85981	4.43849
B	5.39149	7.25463	2.72468

B	5.35716	4.75783	8.54814
B	2.67330	8.82217	6.85602
B	2.69604	6.30286	0.32958
B	2.66536	5.71822	10.97038
O	-0.02438	0.04483	7.68428
O	2.66910	1.57109	11.79985
O	0.02399	3.09825	3.59366
O	2.64418	1.58548	8.76140
O	-0.00092	3.11263	0.55521
O	5.36772	0.01305	7.67630
O	8.06600	1.56836	11.79579
O	5.40884	3.10978	3.55422
O	8.05040	1.56826	8.77800
O	5.39325	3.10967	0.53644
O	-2.73738	4.69253	7.71182
O	-0.03054	6.24110	11.81862
O	-2.69403	7.77156	3.57706
O	-0.03826	6.25466	8.80083
O	-2.70173	7.78512	0.55927
O	2.64414	4.66685	7.68428
O	5.36493	6.23920	11.79985
O	2.69319	7.78172	3.58028
O	2.69255	4.63890	4.67078
O	5.36559	6.23882	8.77478
O	2.69387	7.78134	0.55521
O	-2.69954	4.67068	4.67876
O	5.40555	-0.00880	4.64325
O	0.02402	0.01688	4.67078
C	0.74025	2.68471	7.11506
C	1.92792	1.99901	5.24000

Structure A7) Two Carbon Atoms Replacing One Equatorial Boron and its Adjacent Oxygen

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1198.315554 eV
direct lattice vectors
10.796212936 -0.002627393 -0.001369334
-5.400381846 9.353732303 -0.000000084
-0.001559589 -0.000900066 12.305156434

length of vectors
10.796213342 10.800760717 12.305156565

Positions in Cartesian Coordinates
B 143
O 23
C 2

168

B	-1.42809	3.93072	7.88222
B	-0.90423	3.62753	9.59120
B	3.98261	0.81636	11.98191
B	4.50588	0.51547	1.38639
B	1.28595	2.37919	3.78074
B	1.81325	2.07950	5.49338
B	-0.01051	1.47541	7.88222
B	-0.01115	2.08068	9.59120
B	2.69922	3.04054	11.97762
B	2.69884	3.64551	1.38313
B	0.00285	4.60159	3.78074
B	2.69998	0.52751	5.48864
B	0.86632	3.61852	9.60878
B	1.41693	0.81726	11.98341
B	0.89380	0.51669	1.38740
B	-1.28114	2.37868	3.77590
B	3.59972	2.06979	5.49075
B	4.11522	0.74048	4.42479
B	3.59233	1.04394	2.71702
B	1.40279	2.30297	8.52406
B	0.87176	2.59391	6.81298
B	-1.28319	3.86061	0.32471
B	-1.80981	4.16432	10.92220
B	1.28364	0.74328	4.42873
B	1.80695	1.04529	2.71869
B	3.99994	2.29524	8.51552
B	-0.90725	2.59455	6.82468
B	1.28328	3.85925	0.31898
B	1.81026	4.16350	10.91133
B	2.70290	3.19716	4.43011
B	2.70022	2.59151	2.71703
B	2.69437	0.07961	8.52296
B	-0.01830	4.13553	6.81298
B	0.00122	1.63594	0.32471
B	0.00093	1.02802	10.92220
B	3.96006	3.90828	7.86165
B	4.50904	3.62418	9.58163
B	9.37937	0.81474	11.98139
B	9.90473	0.51361	1.38441
B	6.68207	2.37623	3.77725
B	7.20764	2.07375	5.48529
B	5.40571	1.47258	7.88122
B	5.40133	2.07894	9.59051
B	8.09509	3.03918	11.98139

B	8.09698	3.64473	1.38441
B	5.39781	4.60038	3.77909
B	8.09955	0.52892	5.48529
B	6.81171	3.92925	7.87980
B	6.29148	3.63113	9.58592
B	6.81278	0.81589	11.98331
B	6.29170	0.51504	1.38652
B	4.11602	2.37654	3.78053
B	8.99081	2.07337	5.48025
B	9.51516	0.73955	4.42215
B	8.99134	1.04232	2.71446
B	6.81381	2.29662	8.52925
B	6.30074	2.59431	6.81787
B	4.11418	3.85934	0.31902
B	3.59429	4.15704	10.91114
B	6.68321	0.74108	4.42440
B	7.20548	1.04261	2.71587
B	9.36889	2.29166	8.52993
B	4.52258	2.58249	6.81703
B	6.68072	3.85825	0.32159
B	7.20166	4.15917	10.91719
B	8.09786	3.19438	4.42215
B	8.09815	2.58936	2.71446
B	8.09565	0.07641	8.52925
B	5.40253	4.13842	6.81627
B	5.39880	1.63506	0.32385
B	5.39867	1.02941	10.92118
B	-4.11728	8.60979	7.87951
B	-3.59546	8.30934	9.58762
B	1.28222	5.49485	11.97762
B	1.80596	5.19203	1.38313
B	-1.41672	7.05333	3.77946
B	-0.89374	6.75202	5.48864
B	-2.70329	6.16069	7.87951
B	-2.70258	6.76282	9.58762
B	-0.00228	7.71838	11.98191
B	-0.00122	8.32200	1.38639
B	-2.70094	9.27768	3.77946
B	0.00695	5.20809	5.49338
B	-1.28471	8.61244	7.87932
B	-1.80772	8.31048	9.58783
B	-1.28433	5.49599	11.98341
B	-1.80620	5.19323	1.38740
B	-3.98346	7.05432	3.77851
B	0.89178	6.76008	5.49075
B	1.41971	5.41972	4.43012

B 0.89386 5.72023 2.71703
B -1.28444 6.97111 8.52296
B -1.80930 7.27922 6.81751
B -3.98323 8.53668 0.32424
B -4.50725 8.83712 10.92008
B -1.41505 5.41755 4.42873
B -0.89185 5.71975 2.71869
B 1.28714 6.99396 8.51552
B -3.59476 7.27874 6.81666
B -1.41680 8.53618 0.32394
B -0.89532 8.83726 10.92044
B -0.00169 7.87117 4.42479
B -0.00033 7.26660 2.71702
B -0.00475 4.74089 8.52406
B -2.70161 8.82475 6.81751
B -2.69958 6.31334 0.32424
B -2.70140 5.70930 10.92008
B 1.27758 8.62271 7.88122
B 1.80051 8.31574 9.59051
B 6.67906 5.49238 11.98019
B 7.20389 5.19122 1.38467
B 3.98238 7.05198 3.77909
B 4.50245 6.75356 5.48963
B 2.66413 6.15290 7.86165
B 2.69258 6.77038 9.58163
B 5.39550 7.71557 11.98019
B 5.39711 8.32067 1.38467
B 2.69834 9.27625 3.77725
B 5.39941 5.19998 5.48963
B 4.10812 8.61201 7.87980
B 3.58982 8.31054 9.58592
B 4.11160 5.49218 11.97479
B 3.59198 5.19218 1.38224
B 1.41558 7.05383 3.78053
B 6.28863 6.74909 5.48590
B 6.81227 5.41750 4.42473
B 6.29001 5.71896 2.71500
B 4.09841 6.97557 8.51165
B 3.58467 7.28704 6.81627
B 1.41484 8.53548 0.32385
B 0.89026 8.83820 10.92118
B 3.98394 5.41848 4.42907
B 4.50405 5.71876 2.71544
B 6.66905 6.96872 8.52353
B 1.79723 7.30295 6.81703
B 3.98114 8.53407 0.32159

B	4.50221	8.83475	10.91719
B	5.39726	7.86837	4.42473
B	5.39720	7.26534	2.71500
B	5.38966	4.73906	8.51165
B	2.69654	8.83697	6.81787
B	2.69881	6.31084	0.31902
B	2.69668	5.71175	10.91114
O	10.79761	0.00181	7.65592
O	2.69871	1.55788	11.75723
O	0.00292	3.12003	3.55791
O	2.68527	1.57538	8.72664
O	0.00020	3.11846	0.54389
O	5.39551	-0.00238	7.65654
O	8.09703	1.55734	11.75953
O	5.39914	3.11679	3.55583
O	8.09852	1.55821	8.75531
O	5.39777	3.11769	0.54391
O	8.10018	4.67388	7.65591
O	-0.00205	6.23573	11.75723
O	-2.69939	7.79568	3.55690
O	0.00638	6.21535	8.72664
O	-2.70038	7.79510	0.54663
O	5.39670	6.23413	11.75814
O	2.69822	7.79492	3.55583
O	2.70026	4.67734	4.64668
O	5.38666	6.22834	8.73358
O	2.69831	7.79328	0.54391
O	8.09791	4.67526	4.64727
O	5.39922	-0.00023	4.64699
O	10.79766	-0.00085	4.64727
C	1.36039	3.90377	7.88981
C	2.61195	4.62636	7.71294

Structure A8) Two Carbon Atoms Replacing O-O Chain + Oxygen Interstitial (C_O-O_i-C_O)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1201.469439 eV
energy-cutoff : 500.00
volume of cell : 1250.16
direct lattice vectors
10.810225193 -0.000102665 0.000121487
-5.405147652 9.389276176 0.010108736
0.000133121 0.013367696 12.316952927

length of vectors
10.810225194 10.833938824 12.316960182

Positions in Cartesian Coordinates
B 144
O 23
C 2

169

B	-1.42801	3.95645	7.89827
B	-0.89889	3.65571	9.61195
B	3.98617	0.83264	11.99044
B	4.51040	0.50926	1.37667
B	1.28278	2.35751	3.76802
B	1.80438	2.03408	5.47839
B	-0.00937	1.49983	7.89432
B	-0.00241	2.10654	9.60867
B	2.70214	3.06990	11.99583
B	2.70201	3.65349	1.38859
B	0.00155	4.63101	3.80069
B	2.70209	0.49829	5.47365
B	1.38542	3.93352	7.93014
B	0.88782	3.64979	9.61181
B	1.41816	0.83268	11.99038
B	0.89368	0.50927	1.37661
B	-1.27849	2.39767	3.78730
B	3.59984	2.03411	5.47847
B	4.11967	0.72529	4.40908
B	3.59614	1.02842	2.70013
B	1.41021	2.31219	8.53333
B	0.87898	2.60178	6.81964
B	-1.28219	3.87420	0.32797
B	-1.81159	4.19056	10.93734
B	1.28448	0.72526	4.40904
B	1.80801	1.02840	2.70009
B	3.99418	2.31204	8.53365
B	-0.91530	2.61709	6.83460
B	1.28667	3.87500	0.32880
B	1.80792	4.19114	10.93486
B	2.70207	3.14377	4.36332
B	2.70208	2.57747	2.70157
B	2.70209	0.08988	8.52890
B	-0.02496	4.16676	6.83537
B	-0.00035	1.63882	0.32229
B	-0.00314	1.04391	10.92966
B	4.01890	3.93339	7.93068
B	4.51656	3.64962	9.61206
B	9.39046	0.83252	11.99553

B	9.91409	0.51680	1.38657
B	6.68270	2.39756	3.78743
B	7.21650	2.09791	5.49358
B	5.41360	1.49973	7.89454
B	5.40678	2.10640	9.60889
B	8.10728	3.06743	12.00191
B	8.10717	3.66015	1.39149
B	5.40245	4.63083	3.80096
B	8.10724	0.55437	5.49282
B	6.83228	3.95635	7.89847
B	6.30328	3.65553	9.61216
B	6.82409	0.83255	11.99552
B	6.30023	0.51685	1.38656
B	4.12138	2.35749	3.76812
B	8.99796	2.09788	5.49354
B	9.52866	0.75614	4.42616
B	9.00102	1.05653	2.71739
B	6.82944	2.32227	8.54699
B	6.31958	2.61696	6.83480
B	4.11736	3.87498	0.32886
B	3.59641	4.19111	10.93495
B	6.68578	0.75615	4.42616
B	7.21341	1.05655	2.71738
B	9.38511	2.32228	8.54690
B	4.52529	2.60170	6.81990
B	6.68624	3.87409	0.32810
B	7.21594	4.19043	10.93752
B	8.10722	3.21852	4.42564
B	8.10720	2.60891	2.72112
B	8.10725	0.10535	8.54111
B	5.42919	4.16657	6.83561
B	5.40444	1.63875	0.32241
B	5.40748	1.04383	10.92984
B	-4.12252	8.65672	7.89909
B	-3.59637	8.35268	9.60743
B	1.28669	5.52754	12.00147
B	1.80945	5.20901	1.40088
B	-1.42222	7.08376	3.77790
B	-0.91540	6.79967	5.49361
B	-2.70310	6.19310	7.89993
B	-2.70307	6.79917	9.60657
B	0.00157	7.76152	11.99994
B	0.00034	8.35450	1.39289
B	-2.70309	9.29619	3.76821
B	-0.02428	5.24798	5.51258
B	-1.28364	8.65672	7.89910

B	-1.80977	8.35267	9.60746
B	-1.28189	5.52844	12.00416
B	-1.80876	5.21239	1.39707
B	-3.98399	7.08376	3.77792
B	0.87233	6.81824	5.50237
B	1.39445	5.49300	4.45629
B	0.90389	5.75102	2.74053
B	-1.27955	7.01460	8.53639
B	-1.81378	7.31755	6.83183
B	-3.98833	8.56749	0.32664
B	-4.51182	8.88436	10.93698
B	-1.42435	5.45073	4.43392
B	-0.88921	5.74719	2.72361
B	1.28338	7.04971	8.53829
B	-3.59244	7.31757	6.83185
B	-1.41793	8.56747	0.32671
B	-0.89422	8.88434	10.93704
B	-0.01165	7.91341	4.42775
B	0.00213	7.29674	2.72031
B	-0.00520	4.77866	8.54146
B	-2.70311	8.86413	6.82941
B	-2.70310	6.33558	0.32966
B	-2.70298	5.74443	10.93788
B	1.28007	8.68090	7.90807
B	1.80888	8.36528	9.61386
B	6.68619	5.52833	12.00430
B	7.21280	5.21226	1.39725
B	3.99412	7.10079	3.79788
B	4.53165	6.81809	5.50245
B	2.70191	6.27754	7.87504
B	2.70202	6.81197	9.59225
B	5.40264	7.76145	12.00001
B	5.40364	8.35441	1.39297
B	2.70206	9.32425	3.79791
B	5.42838	5.24780	5.51277
B	4.12404	8.68084	7.90810
B	3.59523	8.36526	9.61387
B	4.11760	5.52752	12.00151
B	3.59457	5.20898	1.40091
B	1.40985	7.10098	3.79776
B	6.31941	6.79951	5.49373
B	6.82840	5.45065	4.43413
B	6.29322	5.74704	2.72378
B	4.12065	7.04964	8.53837
B	3.60025	7.37335	6.82230
B	1.41936	8.56793	0.33361

B	0.89669	8.88758	10.94310
B	4.00956	5.49273	4.45643
B	4.50013	5.75086	2.74063
B	6.68359	7.01449	8.53652
B	1.80376	7.37344	6.82228
B	3.98461	8.56788	0.33362
B	4.50751	8.88754	10.94311
B	5.41570	7.91326	4.42787
B	5.40188	7.29660	2.72042
B	5.40954	4.77849	8.54179
B	2.70204	8.91495	6.83825
B	2.70201	6.33257	0.33081
B	2.70214	5.74636	10.92864
O	0.00277	0.02139	7.68207
O	2.70217	1.57989	11.77334
O	0.00725	3.14069	3.58131
O	2.70210	1.57118	8.75269
O	-0.00115	3.12538	0.54329
O	5.40141	0.02132	7.68218
O	8.10729	1.58175	11.77789
O	5.39698	3.14057	3.58137
O	8.10730	1.58130	8.78167
O	5.40517	3.12533	0.54338
O	-2.70298	4.70859	7.68205
O	-0.00083	6.27469	11.78315
O	-2.70311	7.81627	3.53657
O	0.00696	6.27134	8.73924
O	-2.70314	7.82125	0.54633
O	5.40515	6.27462	11.78323
O	2.70206	7.84151	3.58348
O	5.39708	6.27124	8.73936
O	2.70198	7.82072	0.55325
O	-2.70307	4.70228	4.64832
O	0.00296	9.39131	4.64386
O	5.40112	9.39119	4.64396
O	2.70259	4.35356	6.20583
C	2.70261	4.78152	7.52046
C	2.70157	4.63639	4.85548

Structure A9) Two Carbon Atoms Replacing O-O Chain + Boron Interstitial (C_O-B_i-C_O)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1203.861754 eV
energy-cutoff : 500.00
volume of cell : 1250.82
direct lattice vectors

10.832765634 -0.000002107 -0.000000068
-5.416384543 9.381449383 0.000000025
0.000000217 -0.000000112 12.307974744

length of vectors
10.832765634 10.832765761 12.307974744

Positions in Cartesian Coordinates
B 145
O 22
C 2

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B	-1.43685	3.94015	7.89041
B	-0.90534	3.64314	9.59622
B	3.99472	0.82119	11.98551
B	4.52060	0.51677	1.38426
B	1.28761	2.36469	3.78811
B	1.80204	2.03510	5.49138
B	-0.01473	1.47696	7.89042
B	-0.00619	2.08576	9.59622
B	2.70766	3.05429	11.98197
B	2.70766	3.65280	1.39291
B	-0.01688	4.62414	3.78811
B	2.70766	0.50235	5.48716
B	1.37370	3.92069	7.88523
B	0.87919	3.63519	9.59416
B	1.42061	0.82119	11.98551
B	0.89472	0.51678	1.38426
B	-1.28452	2.38597	3.77888
B	3.61329	2.03510	5.49138
B	4.12979	0.72624	4.41756
B	3.60682	1.03803	2.71175
B	1.40317	2.29798	8.51988
B	0.86051	2.57869	6.81659
B	-1.28710	3.87063	0.32244
B	-1.81367	4.17386	10.92368
B	1.28554	0.72624	4.41756
B	1.80851	1.03803	2.71175
B	4.01215	2.29798	8.51987
B	-0.91970	2.59660	6.82080
B	1.29035	3.87257	0.32610
B	1.80868	4.17183	10.91515
B	2.70766	3.15054	4.42278
B	2.70766	2.57951	2.71386

B	2.70766	0.08108	8.52907
B	-0.04511	4.14727	6.81659
B	-0.00006	1.64140	0.32244
B	-0.00073	1.03377	10.92368
B	4.04162	3.92069	7.88523
B	4.53613	3.63519	9.59416
B	9.41222	0.81998	11.99045
B	9.93925	0.51570	1.38992
B	6.69984	2.38597	3.77888
B	7.23309	2.07810	5.48473
B	5.43005	1.47696	7.89041
B	5.42151	2.08576	9.59622
B	8.12405	3.05116	11.99045
B	8.12405	3.65972	1.38992
B	5.43221	4.62414	3.78811
B	8.12405	0.53492	5.48473
B	6.85218	3.94015	7.89041
B	6.32066	3.64314	9.59622
B	6.83588	0.81998	11.99045
B	6.30884	0.51570	1.38992
B	4.12771	2.36469	3.78811
B	9.01500	2.07810	5.48473
B	9.54387	0.74397	4.42371
B	9.02002	1.04641	2.71692
B	6.84483	2.30226	8.53674
B	6.33502	2.59660	6.82080
B	4.12498	3.87257	0.32610
B	3.60664	4.17183	10.91515
B	6.70423	0.74397	4.42371
B	7.22807	1.04641	2.71692
B	9.40326	2.30226	8.53674
B	4.55481	2.57869	6.81659
B	6.70243	3.87063	0.32244
B	7.22899	4.17386	10.92368
B	8.12405	3.20317	4.42371
B	8.12405	2.59829	2.71692
B	8.12405	0.08660	8.53674
B	5.46043	4.14726	6.81659
B	5.41538	1.64140	0.32244
B	5.41606	1.03377	10.92368
B	-4.12854	8.63774	7.88424
B	-3.60470	8.33530	9.59103
B	1.29036	5.50914	11.98198
B	1.80868	5.20988	1.39291
B	-1.42951	7.07945	3.77122
B	-0.91969	6.78511	5.48717

B	-2.70872	6.17854	7.88424
B	-2.70872	6.78342	9.59103
B	-0.00004	7.74031	11.98551
B	-0.00073	8.34795	1.38426
B	-2.70872	9.29511	3.77122
B	-0.04511	5.23444	5.49138
B	-1.28890	8.63774	7.88424
B	-1.81274	8.33530	9.59103
B	-1.28709	5.51107	11.98551
B	-1.81367	5.20784	1.38426
B	-3.98793	7.07945	3.77122
B	0.86052	6.80303	5.49138
B	1.37371	5.46101	4.42278
B	0.87918	5.74653	2.71386
B	-1.28453	6.99575	8.52907
B	-1.81776	7.30361	6.82322
B	-3.99690	8.56174	0.31748
B	-4.52394	8.86602	10.91801
B	-1.43686	5.44156	4.41756
B	-0.90535	5.73857	2.71175
B	1.28761	7.01702	8.51987
B	-3.59968	7.30361	6.82322
B	-1.42054	8.56174	0.31748
B	-0.89351	8.86602	10.91801
B	-0.01473	7.90476	4.41756
B	-0.00620	7.29596	2.71175
B	-0.01688	4.75758	8.51987
B	-2.70872	8.84680	6.82322
B	-2.70872	6.33054	0.31748
B	-2.70872	5.72198	10.91801
B	1.28554	8.65547	7.89041
B	1.80851	8.34367	9.59622
B	6.70242	5.51107	11.98551
B	7.22899	5.20784	1.38426
B	4.01216	7.08373	3.78811
B	4.55480	6.80303	5.49138
B	2.70766	6.23118	7.88523
B	2.70766	6.80219	9.59416
B	5.41537	7.74031	11.98551
B	5.41605	8.34795	1.38426
B	2.70766	9.30062	3.77888
B	5.46043	5.23444	5.49138
B	4.12979	8.65547	7.89041
B	3.60681	8.34367	9.59622
B	4.12497	5.50914	11.98197
B	3.60664	5.20988	1.39291

B	1.40317	7.08374	3.78811
B	6.33501	6.78511	5.48717
B	6.85218	5.44156	4.41756
B	6.32068	5.73857	2.71175
B	4.12771	7.01702	8.51988
B	3.61328	7.34662	6.81659
B	1.42062	8.56053	0.32244
B	0.89473	8.86494	10.92368
B	4.04162	5.46101	4.42278
B	4.53614	5.74653	2.71386
B	6.69985	6.99575	8.52907
B	1.80204	7.34662	6.81659
B	3.99471	8.56053	0.32244
B	4.52059	8.86494	10.92368
B	5.43006	7.90476	4.41756
B	5.42152	7.29596	2.71175
B	5.43220	4.75758	8.51987
B	2.70766	8.87937	6.82080
B	2.70766	6.32743	0.32610
B	2.70766	5.72891	10.91515
B	2.70766	4.69086	6.15403
O	-5.41597	9.38104	7.67044
O	2.70767	1.56418	11.76734
O	0.00277	3.12918	3.57330
O	2.70766	1.56751	8.73466
O	-0.00013	3.12751	0.54067
O	-0.00147	9.38103	7.67044
O	8.12405	1.56370	11.77707
O	5.41256	3.12918	3.57330
O	8.12405	1.56371	8.76557
O	5.41546	3.12751	0.54067
O	-2.70872	4.69195	7.67044
O	-0.00012	6.25419	11.76734
O	-2.70872	7.81800	3.54236
O	0.00276	6.25253	8.73465
O	-2.70872	7.81800	0.53081
O	5.41545	6.25419	11.76734
O	2.70766	7.81420	3.57330
O	5.41256	6.25253	8.73466
O	2.70766	7.81755	0.54067
O	8.12405	4.68976	4.63753
O	5.41680	0.00068	4.63753
O	10.83129	0.00068	4.63753
C	2.70766	4.69086	7.59273
C	2.70766	4.69085	4.71535

Structure A10) Two Carbon Atoms Replacing O-O Chain + Carbon Interstitial (C_O-C_i-C_O)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1205.569649 eV
energy-cutoff : 500.00
volume of cell : 1250.04
direct lattice vectors
10.832105882 -0.000002146 0.000000076
-5.416054745 9.380877937 -0.000000048
0.000000395 -0.000000095 12.301774187

length of vectors
10.832105882 10.832105975 12.301774187

Positions in Cartesian Coordinates
B 144
O 22
C 3

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B	-1.43826	3.93693	7.88522
B	-0.89834	3.64412	9.58967
B	3.99538	0.82014	11.97834
B	4.52116	0.51610	1.38359
B	1.28389	2.36556	3.78865
B	1.80231	2.02513	5.49332
B	-0.01805	1.47706	7.88522
B	-0.00168	2.09106	9.58967
B	2.70750	3.05149	11.97832
B	2.70750	3.65738	1.39105
B	-0.01782	4.62019	3.78865
B	2.70750	0.49286	5.48048
B	1.35012	3.90689	7.86029
B	0.89252	3.64269	9.57965
B	1.41961	0.82014	11.97834
B	0.89384	0.51610	1.38359
B	-1.28712	2.38428	3.77824
B	3.61268	2.02513	5.49332
B	4.12771	0.72342	4.41654
B	3.60417	1.04460	2.71209
B	1.40578	2.29518	8.51315
B	0.85176	2.57394	6.80846
B	-1.28834	3.87068	0.32340
B	-1.81453	4.17400	10.91815
B	1.28729	0.72342	4.41654

B	1.81083	1.04460	2.71209
B	4.00921	2.29518	8.51315
B	-0.92782	2.59172	6.8212
B	1.28801	3.87103	0.32355
B	1.81273	4.17397	10.91082
B	2.70750	3.12321	4.44154
B	2.70750	2.59481	2.72219
B	2.70750	0.07798	8.52350
B	-0.05343	4.14177	6.80846
B	-0.00046	1.64002	0.32340
B	-0.00088	1.03267	10.91815
B	4.06487	3.90689	7.86029
B	4.52248	3.64269	9.57965
B	9.41150	0.82001	11.98018
B	9.93705	0.51658	1.38552
B	6.70211	2.38428	3.77824
B	7.23528	2.07645	5.48117
B	5.43304	1.47706	7.88522
B	5.41667	2.09105	9.58967
B	8.12355	3.05081	11.98017
B	8.12355	3.65766	1.38552
B	5.43282	4.62019	3.78865
B	8.12355	0.53793	5.48117
B	6.85325	3.93693	7.88522
B	6.31333	3.64412	9.58967
B	6.83560	0.82001	11.98017
B	6.31005	0.51658	1.38552
B	4.13111	2.36556	3.78865
B	9.01182	2.07645	5.48117
B	9.54329	0.74392	4.41970
B	9.01857	1.04687	2.71375
B	6.84425	2.30222	8.53732
B	6.34281	2.59172	6.82127
B	4.12699	3.87103	0.32355
B	3.60227	4.17397	10.91082
B	6.70381	0.74392	4.41970
B	7.22853	1.04687	2.71375
B	9.40285	2.30222	8.53732
B	4.56324	2.57394	6.80846
B	6.70334	3.87068	0.32340
B	7.22952	4.17400	10.91815
B	8.12355	3.20298	4.41970
B	8.12355	2.59708	2.71375
B	8.12355	0.08640	8.53732
B	5.46842	4.14177	6.80847
B	5.41546	1.64002	0.32340

B	5.41587	1.03267	10.91815
B	-4.12830	8.63722	7.88205
B	-3.60357	8.33427	9.58800
B	1.28801	5.51011	11.97832
B	1.81273	5.20716	1.39105
B	-1.42925	7.07892	3.76442
B	-0.92783	6.78942	5.48048
B	-2.70856	6.17815	7.88205
B	-2.70856	6.78406	9.58800
B	-0.00045	7.74112	11.97834
B	-0.00087	8.34848	1.38359
B	-2.70856	9.29474	3.76442
B	-0.05344	5.23938	5.49332
B	-1.28881	8.63722	7.88205
B	-1.81354	8.33427	9.58800
B	-1.28833	5.51044	11.97834
B	-1.81453	5.20713	1.38359
B	-3.98786	7.07892	3.76442
B	0.85175	6.80720	5.49332
B	1.35012	5.47425	4.44154
B	0.89252	5.73845	2.72219
B	-1.28712	6.99687	8.52350
B	-1.82029	7.30469	6.82058
B	-3.99652	8.56113	0.32154
B	-4.52208	8.86457	10.91621
B	-1.43826	5.44421	4.41654
B	-0.89834	5.73702	2.71209
B	1.28389	7.01558	8.51315
B	-3.59682	7.30469	6.82058
B	-1.42059	8.56113	0.32154
B	-0.89504	8.86457	10.91621
B	-0.01805	7.90408	4.41654
B	-0.00167	7.29009	2.71209
B	-0.01783	4.76095	8.51315
B	-2.70856	8.84321	6.82058
B	-2.70856	6.33032	0.32154
B	-2.70856	5.72346	10.91621
B	1.28729	8.65772	7.88522
B	1.81084	8.33654	9.58967
B	6.70333	5.51044	11.97834
B	7.22952	5.20712	1.38359
B	4.00921	7.08595	3.78865
B	4.56324	6.80720	5.49332
B	2.70750	6.25794	7.86029
B	2.70750	6.78633	9.57965
B	5.41544	7.74112	11.97834

B	5.41586	8.34848	1.38359
B	2.70750	9.30315	3.77824
B	5.46843	5.23937	5.49332
B	4.12770	8.65772	7.88522
B	3.60416	8.33654	9.58967
B	4.12698	5.51011	11.97832
B	3.60226	5.20716	1.39105
B	1.40579	7.08595	3.78865
B	6.34282	6.78942	5.48048
B	6.85326	5.44421	4.41654
B	6.31333	5.73701	2.71209
B	4.13111	7.01558	8.51315
B	3.61268	7.35600	6.80847
B	1.41962	8.56101	0.32340
B	0.89385	8.86504	10.91815
B	4.06487	5.47425	4.44154
B	4.52248	5.73845	2.72219
B	6.70212	6.99686	8.52350
B	1.80231	7.35600	6.80847
B	3.99537	8.56101	0.32340
B	4.52114	8.86504	10.91815
B	5.43305	7.90408	4.41654
B	5.41666	7.29009	2.71209
B	5.43282	4.76095	8.51315
B	2.70750	8.88827	6.82128
B	2.70750	6.32966	0.32356
B	2.70750	5.72376	10.91082
O	0.00000	0.00015	7.66698
O	2.70750	1.56373	11.75879
O	0.00318	3.12923	3.57830
O	2.70750	1.56788	8.72345
O	-0.00044	3.12714	0.54302
O	5.41557	0.00016	7.66698
O	8.12355	1.56361	11.76272
O	5.41182	3.12923	3.57830
O	8.12355	1.56361	8.78314
O	5.41544	3.12714	0.54302
O	8.12355	4.69052	7.66698
O	-0.00042	6.25399	11.75879
O	-2.70855	7.81753	3.51859
O	0.00316	6.25192	8.72345
O	-2.70855	7.81753	0.53892
O	5.41542	6.25399	11.75879
O	2.70750	7.81325	3.57830
O	5.41183	6.25192	8.72345
O	2.70750	7.81742	0.54302

O -2.70855 4.69061 4.63479
O 5.41549 0.00011 4.63479
O -0.00049 0.00011 4.63479
C 2.70749 4.69057 6.15096
C 2.70750 4.69057 7.47486
C 2.70750 4.69057 4.82706

Structure A11) 1 Carbon Replacing Oxygen, 1 Carbon Interstitial, and 1 Boron Replacing Oxygen (C_O-C_i-B_O)

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1200.990305 eV
energy-cutoff : 500.00
volume of cell : 1253.21
direct lattice vectors
10.845623935 -0.000002537 0.000000036
-5.422814141 9.392585234 0.000000766
0.000000122 0.000001008 12.302277543

length of vectors
10.845623935 10.845624490 12.302277543

Positions in Cartesian Coordinates
B 145
O 22
C 2

169

B -1.438146 3.941161 7.887471
B -0.901583 3.645340 9.593136
B 4.000445 0.821610 11.977950
B 4.525423 0.513096 1.381912
B 1.289690 2.356786 3.791573
B 1.805940 2.008255 5.495053
B -0.017716 1.480905 7.887462
B -0.005619 2.093487 9.593134
B 2.710878 3.056671 11.985096
B 2.710874 3.659032 1.402088
B -0.025899 4.635453 3.791567
B 2.710879 0.473142 5.474751
B 1.364472 3.919084 7.866503
B 0.891839 3.646204 9.581019
B 1.421312 0.821611 11.977949
B 0.896331 0.513100 1.381912
B -1.283228 2.390419 3.783428

B 3.615817 2.008255 5.495051
B 4.132901 0.715512 4.412277
B 3.607991 1.034138 2.706232
B 1.405025 2.301574 8.512904
B 0.858211 2.577695 6.807753
B -1.289802 3.875498 0.322931
B -1.817628 4.176462 10.916944
B 1.288854 0.715513 4.412283
B 1.813758 1.034138 2.706234
B 4.016726 2.301574 8.512907
B -0.927816 2.595633 6.822823
B 1.290929 3.876619 0.326028
B 1.814066 4.178648 10.910048
B 2.710877 3.085678 4.440494
B 2.710875 2.583259 2.725358
B 2.710874 0.082093 8.520550
B -0.050340 4.151346 6.807755
B -0.000407 1.642198 0.322939
B -0.003674 1.034614 10.916948
B 4.057276 3.919083 7.866503
B 4.529912 3.646204 9.581018
B 9.422893 0.821242 11.982424
B 9.948602 0.517716 1.386310
B 6.704983 2.390417 3.783423
B 7.243805 2.079334 5.485424
B 5.439468 1.480904 7.887465
B 5.427368 2.093488 9.593134
B 8.133690 3.054204 11.982421
B 8.133691 3.661238 1.386308
B 5.447651 4.635450 3.791564
B 8.133685 0.538014 5.485428
B 6.859896 3.941158 7.887469
B 6.323331 3.645342 9.593135
B 6.844488 0.821243 11.982424
B 6.318779 0.517715 1.386310
B 4.132064 2.356786 3.791566
B 9.023567 2.079334 5.485426
B 9.557014 0.743799 4.417930
B 9.030033 1.048047 2.713576
B 6.854144 2.304309 8.538927
B 6.349565 2.595629 6.822824
B 4.130826 3.876617 0.326032
B 3.607689 4.178649 10.910048
B 6.710364 0.743800 4.417924
B 7.237350 1.048046 2.713574
B 9.413231 2.304308 8.538926

B	4.563539	2.577691	6.807754
B	6.711557	3.875496	0.322936
B	7.239377	4.176460	10.916945
B	8.133687	3.209066	4.417915
B	8.133693	2.600557	2.713569
B	8.133688	0.088073	8.538924
B	5.472089	4.151342	6.807755
B	5.422162	1.642197	0.322941
B	5.425429	1.034615	10.916948
B	-4.135522	8.649196	7.885552
B	-3.608169	8.344733	9.589153
B	1.290806	5.516303	11.985089
B	1.812466	5.215122	1.402085
B	-1.438399	7.092005	3.757409
B	-0.946600	6.808061	5.474749
B	-2.711937	6.183479	7.885563
B	-2.711941	6.792418	9.589157
B	-0.000030	7.750629	11.977937
B	-0.004714	8.359520	1.381907
B	-2.711937	9.297838	3.757415
B	-0.069624	5.256805	5.495049
B	-1.288354	8.649195	7.885556
B	-1.815710	8.344734	9.589154
B	-1.289595	5.517036	11.977939
B	-1.819258	5.216643	1.381907
B	-3.985475	7.092005	3.757411
B	0.835315	6.824203	5.495054
B	1.315927	5.501790	4.440497
B	0.880824	5.753002	2.725358
B	-1.285259	7.003598	8.520559
B	-1.824693	7.315035	6.820098
B	-4.001341	8.571723	0.316608
B	-4.527108	8.875282	10.914133
B	-1.447706	5.455367	4.412271
B	-0.909310	5.750636	2.706228
B	1.289793	7.024754	8.512915
B	-3.599181	7.315033	6.820097
B	-1.422531	8.571722	0.316606
B	-0.896767	8.875283	10.914132
B	-0.025685	7.918382	4.412278
B	-0.012193	7.304487	2.706231
B	-0.016057	4.762957	8.512915
B	-2.711936	8.851786	6.820096
B	-2.711936	6.338409	0.316607
B	-2.711938	5.731309	10.914131
B	1.290444	8.667215	7.887467

B	1.814912	8.350452	9.593135
B	6.711349	5.517034	11.977945
B	7.241013	5.216641	1.381909
B	4.026465	7.097016	3.791579
B	4.586432	6.824198	5.495056
B	2.710873	6.251117	7.866506
B	2.710876	6.796871	9.581021
B	5.421784	7.750629	11.977941
B	5.426464	8.359520	1.381909
B	2.710876	9.308412	3.783436
B	5.491372	5.256801	5.495049
B	4.131304	8.667215	7.887462
B	3.606839	8.350451	9.593134
B	4.130948	5.516301	11.985093
B	3.609283	5.215123	1.402087
B	1.395286	7.097017	3.791575
B	6.368348	6.808056	5.474751
B	6.869456	5.455363	4.412269
B	6.331059	5.750638	2.706228
B	4.131955	7.024754	8.512910
B	3.619422	7.360241	6.807755
B	1.421479	8.571575	0.322928
B	0.896924	8.878211	10.916944
B	4.105821	5.501787	4.440497
B	4.540925	5.753002	2.725359
B	6.707006	7.003597	8.520556
B	1.802321	7.360242	6.807756
B	4.000273	8.571575	0.322931
B	4.524826	8.878206	10.916945
B	5.447433	7.918379	4.412283
B	5.433943	7.304488	2.706233
B	5.437804	4.762955	8.512912
B	2.710871	8.898016	6.822824
B	2.710875	6.336036	0.326025
B	2.710878	5.731973	10.910047
B	2.710873	4.696420	4.781445
O	-0.000744	0.000260	7.675302
O	2.710881	1.566163	11.765149
O	0.004764	3.134043	3.590001
O	2.710877	1.570108	8.722119
O	-0.000866	3.130797	0.538127
O	5.422499	0.000259	7.675313
O	8.133693	1.565562	11.765956
O	5.416994	3.134041	3.589986
O	8.133689	1.565563	8.783696
O	5.422625	3.130796	0.538135

O -2.711936 4.696181 7.675328
O -0.000008 6.261556 11.765123
O -2.711936 7.827283 3.499347
O 0.003401 6.259589 8.722146
O -2.711934 7.827285 0.531536
O 5.421766 6.261554 11.765134
O 2.710877 7.821167 3.590018
O 5.418350 6.259587 8.722136
O 2.710878 7.827676 0.538113
O 8.133689 4.695204 4.625668
O 5.423332 0.000731 4.625690
O 10.844049 0.000729 4.625704
C 2.710873 4.696425 6.153186
C 2.710874 4.696428 7.504038

Structure A12) C-B-C Chain Replacing O-O Chain + Single Carbon Substitution in Equatorial Boron

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1205.995839 eV
energy-cutoff : 500.00
volume of cell : 1248.53
direct lattice vectors
10.822235010 0.001595664 -0.005400631
-5.409735672 9.369933084 -0.000000303
-0.006144969 -0.003547810 12.311461465

length of vectors
10.822236475 10.819467918 12.311463510

Positions in Cartesian Coordinates
B 144
O 22
C 3

169

B 2.688166 4.675762 6.141358
B -1.445043 3.928720 7.891661
B -0.912456 3.630223 9.600868
B 3.988394 0.817699 11.985741
B 4.517527 0.515820 1.381598
B 1.290792 2.366936 3.783831
B 1.815823 2.047800 5.492524
B -0.025394 1.469817 7.891661
B -0.017608 2.080301 9.600868

B 2.702867 3.045807 11.987080
B 2.707940 3.652395 1.389965
B -0.010022 4.620011 3.783831
B 2.705726 0.502807 5.485812
B 0.865749 3.623590 9.612329
B 1.415787 0.817469 11.988698
B 0.896416 0.515911 1.384011
B -1.281118 2.384094 3.779204
B 3.608573 2.035896 5.487602
B 4.125896 0.726909 4.418732
B 3.602705 1.037205 2.712335
B 1.396317 2.295817 8.534220
B 0.851487 2.580333 6.816419
B -1.284042 3.867756 0.325855
B -1.819089 4.167964 10.931079
B 1.285929 0.730394 4.423208
B 1.810571 1.038618 2.714848
B 4.005658 2.299750 8.518980
B -0.925210 2.589578 6.832261
B 1.290253 3.868674 0.322784
B 1.814635 4.171426 10.916550
B 2.711709 3.152984 4.418181
B 2.707134 2.580083 2.715752
B 2.697350 0.076877 8.527771
B -0.044868 4.132865 6.816419
B 0.002311 1.639728 0.325855
B -0.005224 1.026262 10.931079
B 3.998312 3.909104 7.889380
B 4.519957 3.633364 9.591603
B 9.397854 0.817722 11.986651
B 9.930341 0.518820 1.381682
B 6.694425 2.385484 3.775710
B 7.225481 2.078585 5.483175
B 5.419240 1.475475 7.884450
B 5.409592 2.084654 9.595568
B 8.111588 3.045600 11.986650
B 8.118974 3.656200 1.381682
B 5.432499 4.622929 3.774757
B 8.117339 0.533844 5.483175
B 6.825013 3.936082 7.883908
B 6.304611 3.637038 9.591931
B 6.824581 0.817296 11.987897
B 6.306149 0.517980 1.384040
B 4.125604 2.363801 3.782375
B 9.006620 2.077098 5.477852
B 9.537141 0.743862 4.418511

B	9.012534	1.047425	2.712654
B	6.826345	2.300946	8.534263
B	6.317273	2.596800	6.819048
B	4.124938	3.869275	0.322591
B	3.598250	4.165565	10.918655
B	6.698820	0.744689	4.420218
B	7.223430	1.047572	2.713655
B	9.382691	2.294222	8.538399
B	4.539736	2.578866	6.814846
B	6.699351	3.869321	0.319172
B	7.218685	4.167063	10.921456
B	8.117264	3.203159	4.418511
B	8.117854	2.597054	2.712654
B	8.110341	0.077001	8.534263
B	5.421742	4.148742	6.812072
B	5.412311	1.640726	0.321826
B	5.407796	1.030076	10.925115
B	-4.125998	8.622673	7.886158
B	-3.603436	8.323088	9.594096
B	1.283937	5.503466	11.987081
B	1.811792	5.204566	1.389965
B	-1.425438	7.071517	3.771151
B	-0.916940	6.777445	5.485812
B	-2.710525	6.171000	7.886157
B	-2.708692	6.773344	9.594095
B	-0.002899	7.730819	11.985740
B	0.000232	8.340002	1.381597
B	-2.703583	9.285331	3.771151
B	-0.023888	5.234271	5.492524
B	-1.288378	8.626526	7.885984
B	-1.812456	8.323949	9.593953
B	-1.289402	5.502991	11.988698
B	-1.810244	5.203982	1.384010
B	-3.979621	7.072735	3.769302
B	0.862178	6.792789	5.487603
B	1.381173	5.457539	4.418182
B	0.882740	5.740026	2.715752
B	-1.289995	6.983158	8.527769
B	-1.817313	7.293281	6.824131
B	-3.988862	8.552581	0.320121
B	-4.520355	8.851128	10.924536
B	-1.429742	5.434071	4.423209
B	-0.900490	5.734312	2.714848
B	1.289225	7.004748	8.518978
B	-3.597934	7.293104	6.823401
B	-1.415735	8.552993	0.318807

B	-0.896453	8.852801	10.923588
B	-0.012776	7.895296	4.418731
B	-0.005647	7.287051	2.712335
B	-0.018853	4.746961	8.534219
B	-2.707470	8.835078	6.824131
B	-2.702656	6.324806	0.320120
B	-2.709853	5.715248	10.924535
B	1.282174	8.641082	7.884449
B	1.804914	8.328136	9.595568
B	6.693411	5.503272	11.981859
B	7.228354	5.206679	1.376719
B	4.014580	7.078836	3.774757
B	4.552377	6.789773	5.479755
B	2.679294	6.193709	7.889380
B	2.701318	6.783335	9.591603
B	5.407437	7.730644	11.981859
B	5.418051	8.342216	1.376719
B	2.707858	9.290418	3.775711
B	5.451061	5.233208	5.479756
B	4.116009	8.628213	7.883908
B	3.596828	8.327054	9.591931
B	4.118616	5.501629	11.984080
B	3.605616	5.205449	1.387502
B	1.404667	7.076597	3.782375
B	6.331810	6.779419	5.477148
B	6.848064	5.438762	4.414574
B	6.320733	5.738236	2.705795
B	4.112894	6.991592	8.522900
B	3.598543	7.306616	6.812071
B	1.421822	8.552452	0.321826
B	0.890725	8.853868	10.925115
B	4.049485	5.461718	4.404409
B	4.537992	5.743757	2.707801
B	6.688446	6.985322	8.525230
B	1.797986	7.327715	6.814845
B	3.995363	8.552764	0.319172
B	4.512882	8.853650	10.921456
B	5.428895	7.896835	4.414573
B	5.424582	7.290415	2.705795
B	5.406100	4.751695	8.522900
B	2.702287	8.858139	6.819049
B	2.708117	6.323282	0.322591
B	2.701366	5.719013	10.918654
O	-0.005846	-0.000442	7.669346
O	2.700820	1.560339	11.762491
O	0.005656	3.127012	3.573044

O 2.687063 1.580589 8.728038
O 0.002925 3.125433 0.541317
O 5.405822 -0.001825 7.666507
O 8.112102 1.560644 11.765792
O 5.409500 3.126817 3.566654
O 8.111465 1.560279 8.770024
O 5.413345 3.126599 0.538920
O -2.708551 4.680777 7.669344
O -0.003539 6.244424 11.762490
O -2.701363 7.810736 3.533114
O 0.007113 6.222394 8.728030
O -2.702512 7.810071 0.537363
O 5.406713 6.245310 11.762134
O 2.707409 7.806973 3.566656
O 5.401443 6.242270 8.737293
O 2.709145 7.810410 0.538919
O -2.701184 4.684695 4.644165
O 5.412836 0.002225 4.640766
O 0.001230 0.003978 4.644164
C 2.591852 4.620154 7.590853
C 2.722001 4.695296 4.722328
C 1.310679 3.880469 7.925371

Structure A13) C-B-C Chain Replacing O-O Chain + Single Carbon Substitution in Equatorial Boron

Gamma point optimization in VASP using high precision settings and PBE exchange functional
Total System Energy after Optimization = -1206.261092 eV
energy-cutoff : 500.00
volume of cell : 1248.28
direct lattice vectors
10.824838846 0.001529527 0.013659407
-5.411095655 9.376920969 -0.012268016
0.015554815 -0.007153755 12.296949783

length of vectors
10.824847573 10.826206794 12.296961702

Positions in Cartesian Coordinates
B 144
O 22
C 3

169

B 2.690305 4.623918 6.134008
B -1.417880 3.931044 7.875527
B -0.888289 3.630891 9.583776
B 4.010114 0.813171 11.975032
B 4.518250 0.512942 1.383002
B 1.292117 2.361017 3.777264
B 1.813310 2.034771 5.481297
B -0.000085 1.474923 7.870120
B 0.008528 2.076467 9.581101
B 2.722646 3.045484 11.975032
B 2.704992 3.653864 1.392569
B -0.019156 4.622751 3.772266
B 2.711779 0.500321 5.480116
B 1.391786 3.917721 7.876760
B 0.897484 3.625798 9.579203
B 1.435898 0.813539 11.974556
B 0.893480 0.513814 1.382706
B -1.280650 2.390584 3.768385
B 3.613050 2.035362 5.485332
B 4.128873 0.725333 4.416143
B 3.604875 1.032842 2.709765
B 1.418673 2.291910 8.510903
B 0.877385 2.579615 6.806030
B -1.287867 3.870703 0.322691
B -1.798570 4.163181 10.912516
B 1.292605 0.728368 4.415900
B 1.812387 1.033135 2.709138
B 4.025902 2.288858 8.522011
B -0.904035 2.590523 6.809822
B 1.289139 3.870544 0.321667
B 1.827194 4.162101 10.903231
B 2.709776 3.142065 4.407056
B 2.709050 2.574246 2.710319
B 2.723731 0.078492 8.525165
B -0.024405 4.139966 6.804666
B 0.000781 1.640924 0.321515
B 0.015117 1.024484 10.912116
B 4.056772 3.906759 7.888001
B 4.549481 3.624175 9.590380
B 9.421394 0.814510 11.986493
B 9.929888 0.519648 1.394223
B 6.695785 2.389733 3.790474
B 7.238713 2.068295 5.491416
B 5.442704 1.473236 7.883091
B 5.437996 2.077623 9.592560
B 8.133492 3.045783 11.989092

B	8.114838	3.661833	1.397389
B	5.418449	4.633807	3.809178
B	8.135664	0.529226	5.474000
B	6.864512	3.929673	7.886803
B	6.334705	3.630965	9.596567
B	6.848815	0.813774	11.984250
B	6.305139	0.517442	1.391376
B	4.126290	2.361520	3.781415
B	9.016840	2.077162	5.487144
B	9.542495	0.751462	4.417840
B	9.012005	1.054112	2.718348
B	6.854358	2.294359	8.534829
B	6.344691	2.588937	6.824607
B	4.123019	3.872252	0.331390
B	3.620768	4.162671	10.910701
B	6.700582	0.743033	4.424414
B	7.221723	1.053524	2.720123
B	9.415771	2.296127	8.536631
B	4.562331	2.574637	6.814237
B	6.696242	3.871819	0.335419
B	7.242557	4.164626	10.925786
B	8.119268	3.205901	4.433945
B	8.117270	2.603768	2.725450
B	8.138556	0.079854	8.533112
B	5.464639	4.134381	6.823611
B	5.411978	1.640221	0.328393
B	5.433579	1.024095	10.919078
B	-4.099613	8.626107	7.869610
B	-3.583029	8.324881	9.576160
B	1.305302	5.499439	11.968017
B	1.806991	5.206657	1.386524
B	-1.430470	7.075342	3.764730
B	-0.906412	6.781708	5.474864
B	-2.687923	6.166451	7.869750
B	-2.688690	6.772516	9.577784
B	0.018146	7.728868	11.965612
B	-0.002782	8.345696	1.373493
B	-2.703615	9.288839	3.756232
B	-0.033592	5.230932	5.477771
B	-1.270699	8.626934	7.866803
B	-1.792879	8.325149	9.574145
B	-1.271856	5.500851	11.970186
B	-1.819028	5.209012	1.379283
B	-3.994980	7.080925	3.778480
B	0.876656	6.787389	5.463599
B	1.370736	5.453854	4.398844

B 0.872763 5.743500 2.703288
B -1.266851 6.988072 8.510322
B -1.801918 7.296884 6.808923
B -3.993064 8.557012 0.313101
B -4.500096 8.853283 10.903432
B -1.434824 5.440513 4.416688
B -0.910406 5.739120 2.706199
B 1.308806 7.007191 8.506345
B -3.578251 7.299369 6.814371
B -1.417258 8.557822 0.309811
B -0.873814 8.853449 10.901704
B -0.011870 7.899818 4.406533
B -0.014666 7.290814 2.700774
B 0.002431 4.743825 8.509306
B -2.688922 8.840064 6.806176
B -2.708122 6.328621 0.316454
B -2.690473 5.712725 10.907674
B 1.307548 8.642306 7.874431
B 1.831908 8.334048 9.577631
B 6.713760 5.502216 11.982807
B 7.220006 5.212016 1.397531
B 3.994011 7.091439 3.802744
B 4.519919 6.815930 5.546683
B 2.729634 6.216492 7.868757
B 2.727178 6.788896 9.572234
B 5.428620 7.729419 11.979053
B 5.411645 8.347479 1.392320
B 2.706805 9.301626 3.760885
B 5.436508 5.245328 5.519198
B 4.154033 8.642874 7.873321
B 3.625172 8.334052 9.579029
B 4.140574 5.500648 11.978827
B 3.599221 5.209918 1.402854
B 1.397284 7.077753 3.763408
B 6.315145 6.796017 5.511943
B 6.835474 5.448831 4.444585
B 6.308763 5.745320 2.733454
B 4.153253 6.999557 8.527498
B 1.420904 8.557060 0.319841
B 0.914736 8.856215 10.909161
B 4.021551 5.468323 4.448977
B 4.524342 5.750518 2.739737
B 6.720455 6.991426 8.524496
B 1.827794 7.328000 6.789402
B 3.992776 8.557205 0.324584
B 4.540596 8.857119 10.912960

B	5.413190	7.915404	4.442991
B	5.412698	7.296617	2.733329
B	5.443707	4.734726	8.520022
B	2.731838	8.862083	6.797050
B	2.706510	6.326097	0.323610
B	2.726154	5.711861	10.900968
O	10.832896	-0.020999	7.650841
O	2.723106	1.555878	11.755430
O	0.006088	3.127675	3.561813
O	2.720973	1.560656	8.732125
O	-0.000692	3.126491	0.540161
O	5.439630	-0.013395	7.657303
O	8.135237	1.558017	11.766287
O	5.409675	3.137681	3.590983
O	8.136600	1.545778	8.760971
O	5.410640	3.125806	0.550194
O	-2.690068	4.682893	7.653923
O	0.016292	6.243396	11.746774
O	-2.713575	7.810281	3.536184
O	0.030488	6.248260	8.708861
O	-2.705369	7.815904	0.530506
O	5.427952	6.245524	11.754442
O	2.701749	7.815137	3.558822
O	5.414412	6.249434	8.698610
O	2.706685	7.814676	0.540225
O	8.111363	4.694195	4.660756
O	5.417573	-0.000765	4.641958
O	-0.001014	0.009356	4.639924
C	2.735395	4.692330	7.560837
C	2.694361	4.680742	4.713253
C	3.597190	7.352893	6.853087

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